LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121721\
Data File : BM033500.D
Acq On : 17 Dec 2021 11:20
Operator : CG/JU
Sample : M5089-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-2

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM033500.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.037	294	306	314	rBV	242431	356428	3.02%	0.684%
2	5.502	379	385	397	rBV	860525	1270413	10.76%	2.438%
3	7.113	651	659	672	rBV	845985	1428494	12.09%	2.741%
4	7.937	792	799	805	rVB	149238	241940	2.05%	0.464%
5	9.107	990	998	1012	rBV	560574	939036	7.95%	1.802%
6	10.748	1269	1277	1284	rBV	189582	327420	2.77%	0.628%
7	13.207	1688	1695	1702	rBV	1379530	2007552	17.00%	3.852%
8	14.583	1922	1929	1935	rBV	312932	467029	3.95%	0.896%
9	14.889	1947	1981	1982	rBV	151853	814393	6.90%	1.563%
10	15.736	2085	2125	2126	rBV	898239	6308916	53.42%	12.105%
11	16.071	2170	2182	2186	rBV	1667369	3178711	26.91%	6.099%
12	16.354	2226	2230	2246	rVB	5003761	11810828	100.00%	22.662%
13	16.601	2254	2272	2274	rBV	385287	1296141	10.97%	2.487%
14	17.330	2390	2396	2400	rBV	450401	657096	5.56%	1.261%
15	18.218	2532	2547	2556	rBV	524161	1526941	12.93%	2.930%
16	18.554	2600	2604	2616	rVB2	91034	163410	1.38%	0.314%
17	19.383	2737	2745	2756	rBV	140873	254798	2.16%	0.489%
18	19.495	2760	2764	2771	rVV	151046	209585	1.77%	0.402%
19	19.601	2772	2782	2792	rVB	684645	1767123	14.96%	3.391%
20	19.954	2836	2842	2847	rBV	2838028	3444567	29.16%	6.609%
21	20.577	2940	2948	2954	rVB	971374	1834064	15.53%	3.519%
22	20.748	2972	2977	2988	rVB2	218477	466753	3.95%	0.896%
23	21.212	3052	3056	3062	rBV2	167644	230340	1.95%	0.442%
24	21.289	3064	3069	3073	rVV	293807	384545	3.26%	0.738%
25	21.359	3075	3081	3087	rVV	1187065	2077727	17.59%	3.987%
26	21.418	3087	3091	3095	rVB	387796	457439	3.87%	0.878%
27	21.506	3101	3106	3111	rBV2	416069	598998	5.07%	1.149%
28	22.095	3198	3206	3212	rBV	838685	1716066	14.53%	3.293%
29	22.759	3316	3319	3324	rVB	100402	145447	1.23%	0.279%
30	22.900	3336	3343	3352	rBV	704300	1519968	12.87%	2.916%
31	22.995	3352	3359	3370	rVB2	247613	641408	5.43%	1.231%
32	23.153	3380	3386	3396	rBV9	138551	361532	3.06%	0.694%
33	23.824	3493	3500	3509	rVB	484396	1231559	10.43%	2.363%
34	23.924	3512	3517	3528	rVB2	194815	443059	3.75%	0.850%
35	24.889	3673	3681	3694	rVB2	305271	923183	7.82%	1.771%
36	25.741	3821	3826	3843	rVB5	195112	613878	5.20%	1.178%

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121721\
Data File : BM033500.D
Acq On : 17 Dec 2021 11:20
Operator : CG/JU
Sample : M5089-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-2

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

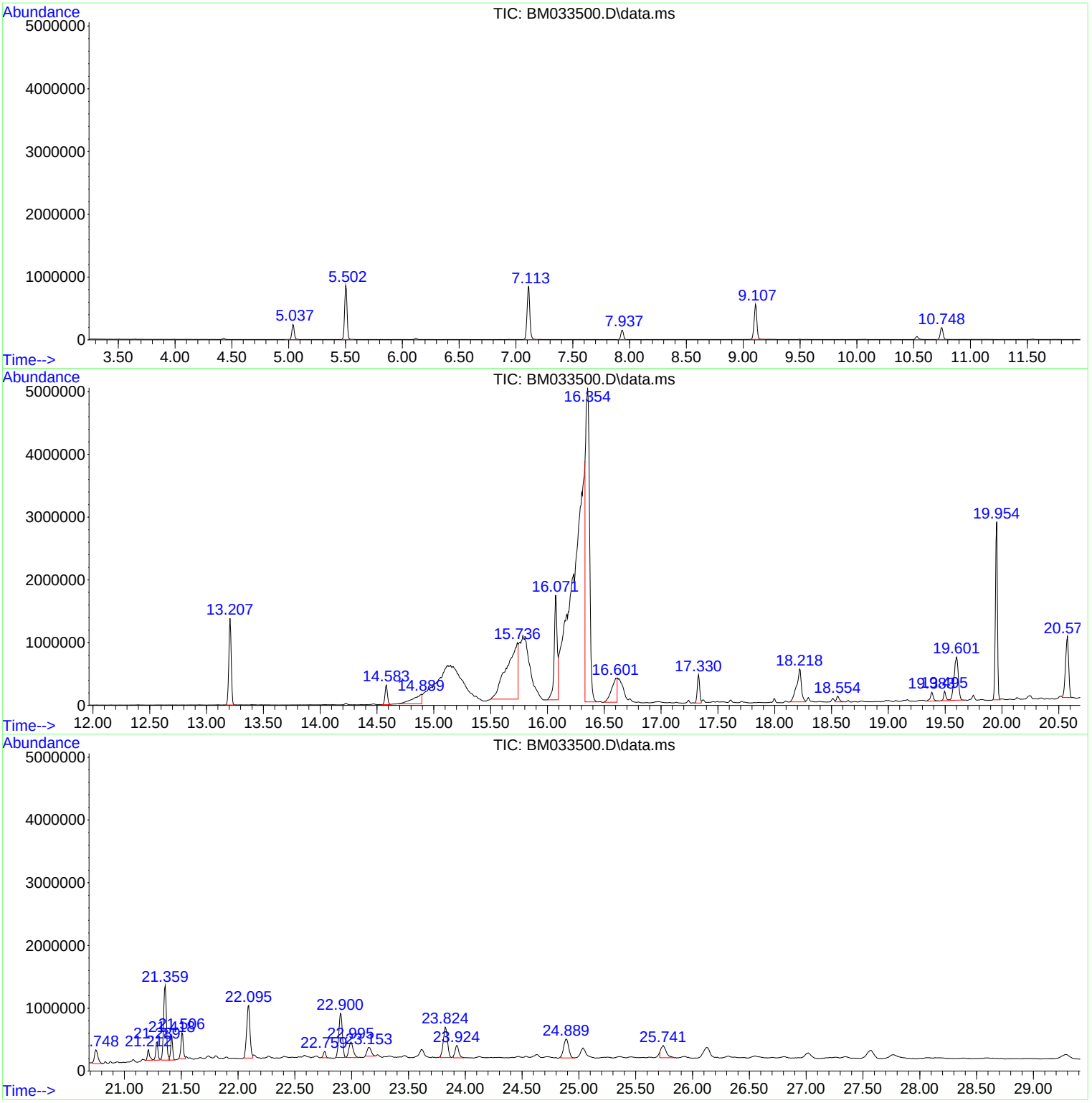
Sum of corrected areas: 52116787

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121721\
Data File : BM033500.D
Acq On : 17 Dec 2021 11:20
Operator : CG/JU
Sample : M5089-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121721\
Data File : BM033500.D
Acq On : 17 Dec 2021 11:20
Operator : CG/JU
Sample : M5089-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-2

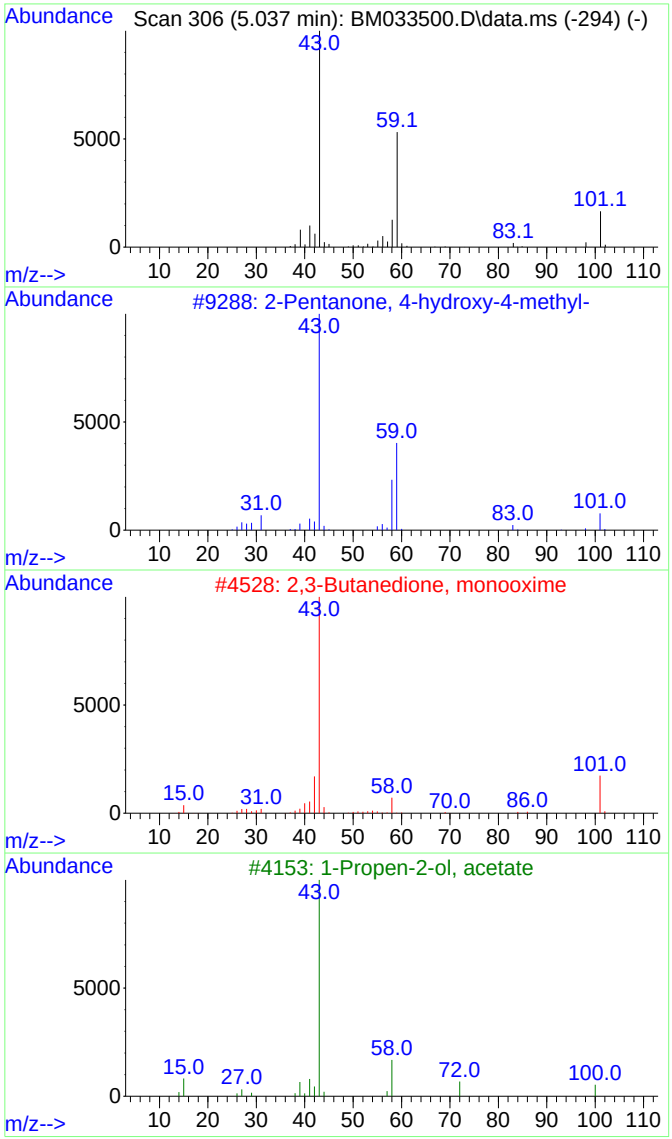
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

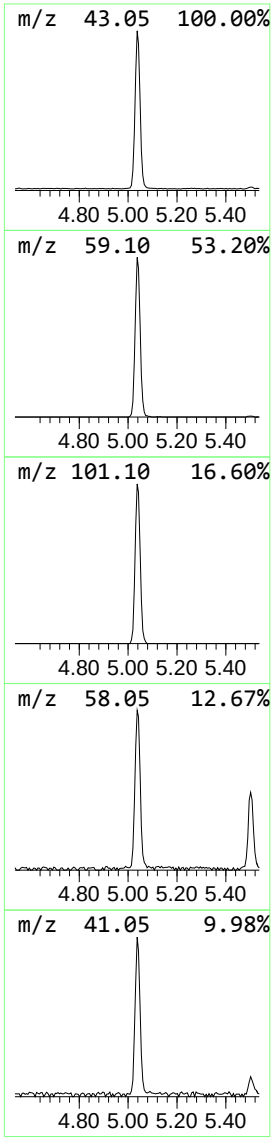
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.037	29.46 ng	356428	1,4-Dichlorobenzene-d4	7.931

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	Acetamide, N-(cyanomethyl)-	98	C4H6N2O	004814-80-6	9
5	2,4-Dimethyl-2,4-pentanediol	132	C7H16O2	024892-49-7	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121721\
Data File : BM033500.D
Acq On : 17 Dec 2021 11:20
Operator : CG/JU
Sample : M5089-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

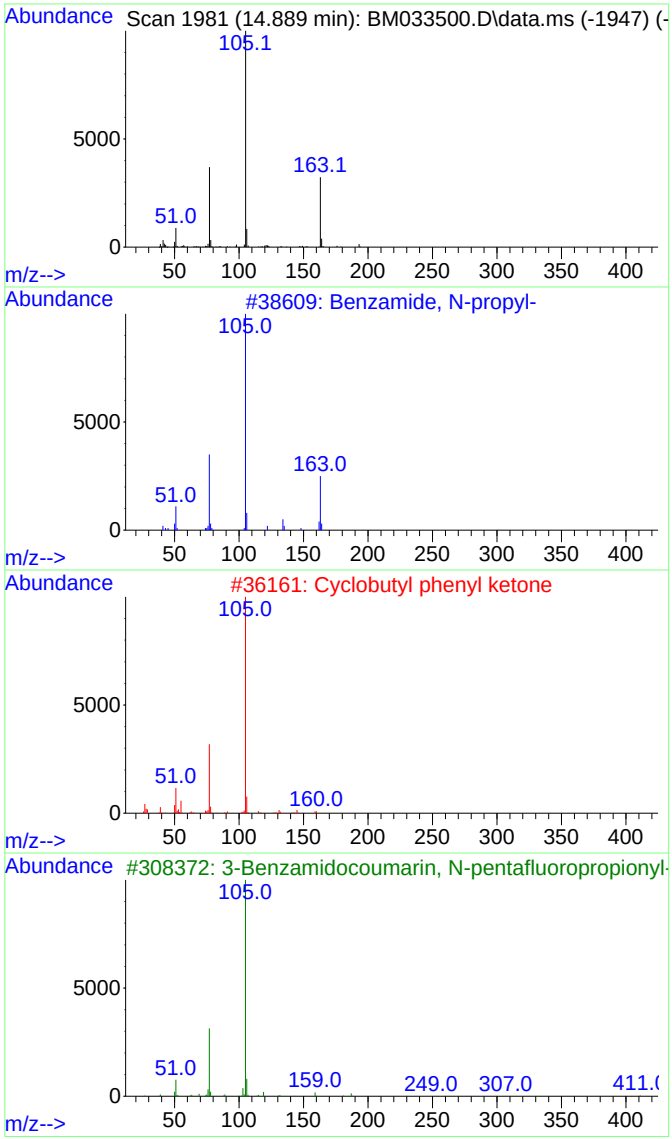
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

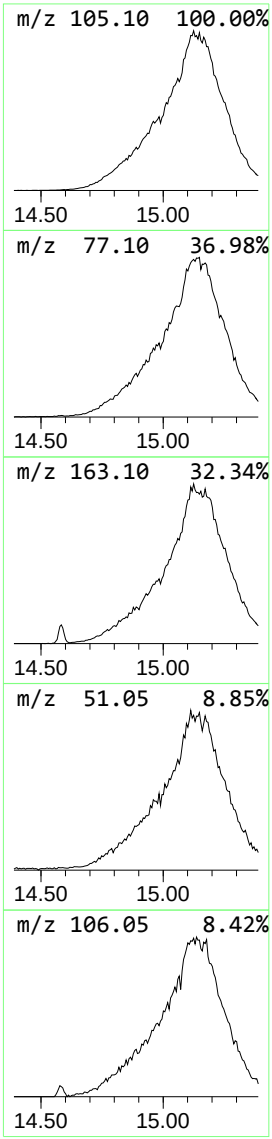
****

Peak Number 2 Benzamide, N-propyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.889	34.88 ng	814393	Acenaphthene-d10	14.583

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzamide, N-propyl-	163	C10H13NO	010546-70-0	83
2	Cyclobutyl phenyl ketone	160	C11H12O	005407-98-7	50
3	3-Benzamidocoumarin, N-pentafluo...	411	C19H10F5NO4	1000446-95-9	47
4	Isopropyl phenyl ketone	148	C10H12O	000611-70-1	47
5	Phenylglyoxylic acid, butyl ester	206	C12H14O3	1000453-46-6	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121721\
Data File : BM033500.D
Acq On : 17 Dec 2021 11:20
Operator : CG/JU
Sample : M5089-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-2

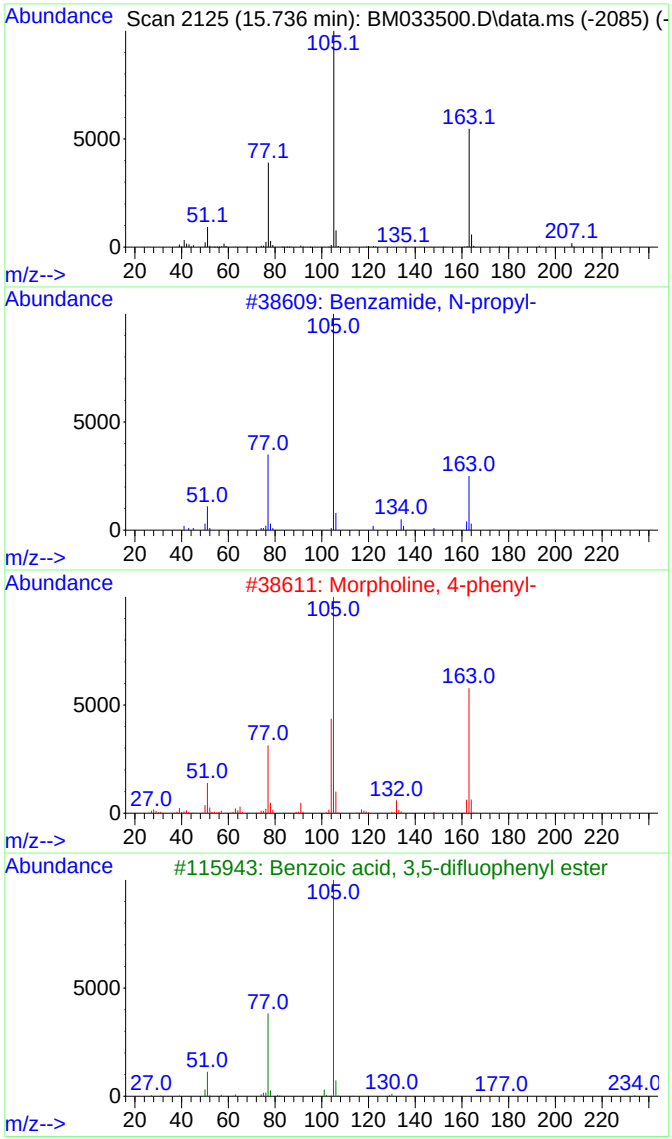
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

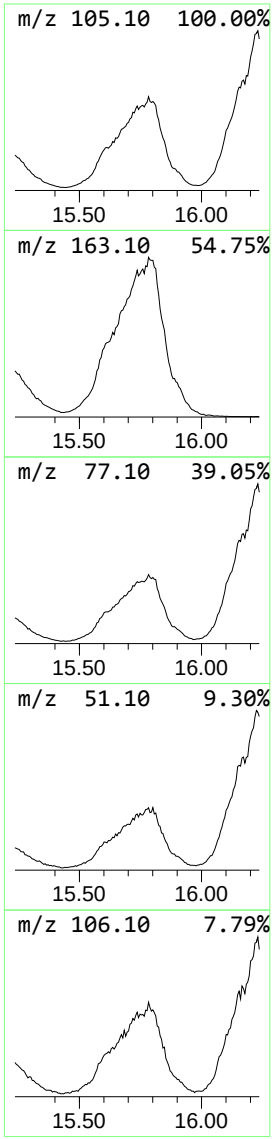
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Morpholine, 4-phenyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.736	270.17 ng	6308920	Acenaphthene-d10	14.583

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzamide, N-propyl-	163	C10H13NO	010546-70-0	72
2	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	72
3	Benzoic acid, 3,5-difluophenyl e...	234	C13H8F2O2	1000357-79-5	47
4	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	47
5	Glycine, N-benzoyl-N-(2,2,3,3,3-...	339	C13H10F5NO4	072347-42-3	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121721\
Data File : BM033500.D
Acq On : 17 Dec 2021 11:20
Operator : CG/JU
Sample : M5089-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

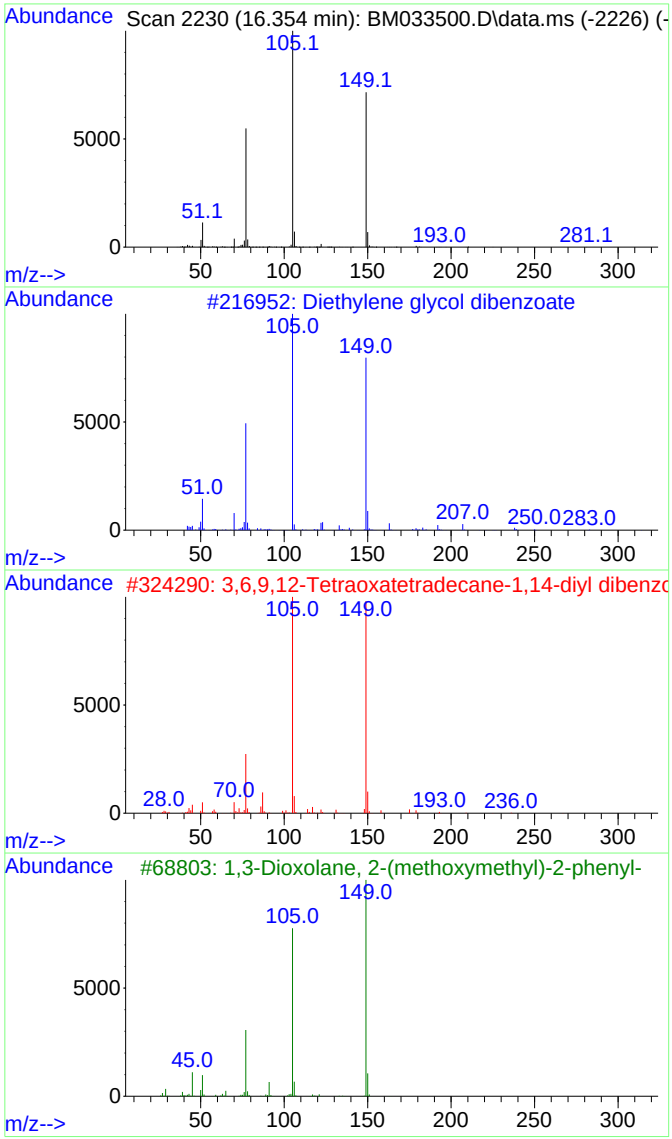
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

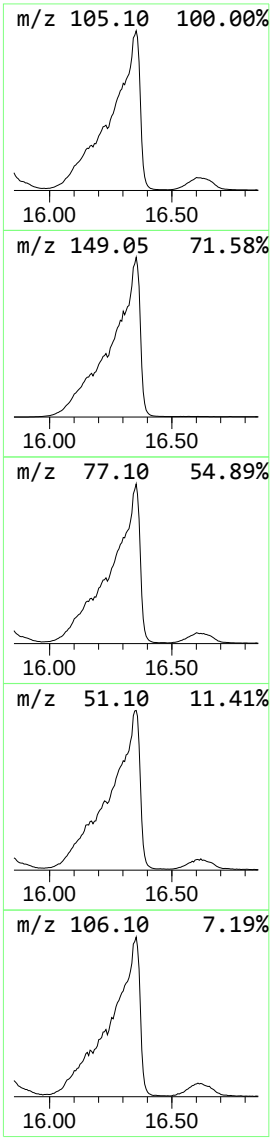
****

Peak Number 4 Diethylene glycol dibenzoate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.354	359.49 ng	11810800	Phenanthrene-d10	17.330

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	83
2	3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	74
3	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	64
4	Phenyl(2-phenyl-1,3-dioxolan-2-y...	270	C17H18O3	1000507-07-6	56
5	Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121721\
Data File : BM033500.D
Acq On : 17 Dec 2021 11:20
Operator : CG/JU
Sample : M5089-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-2

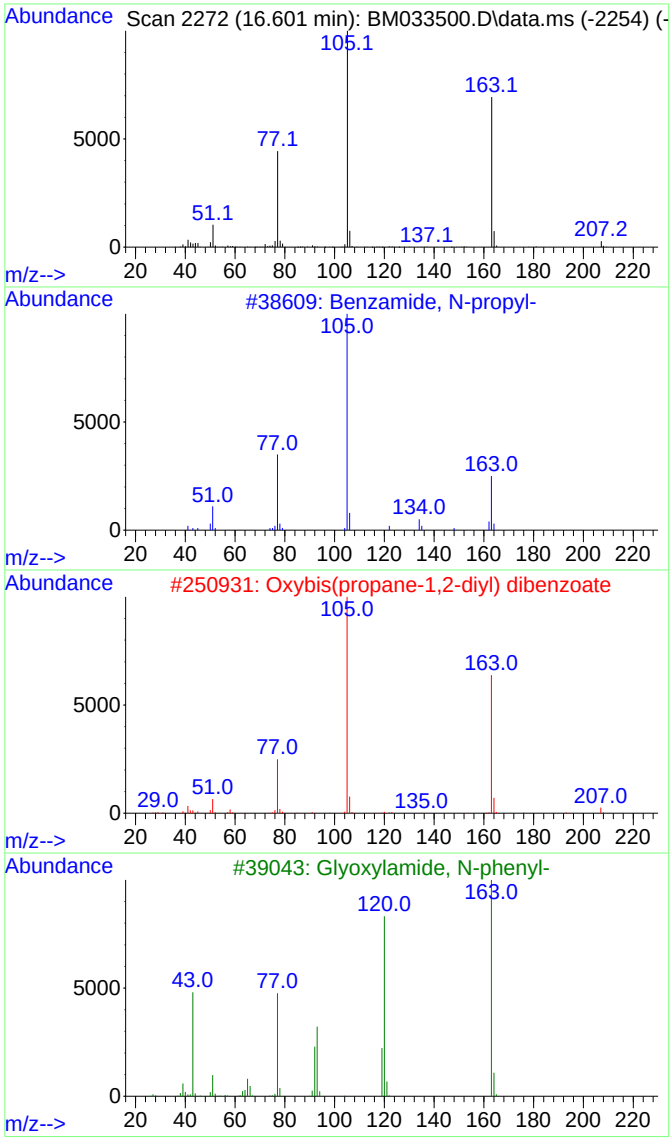
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

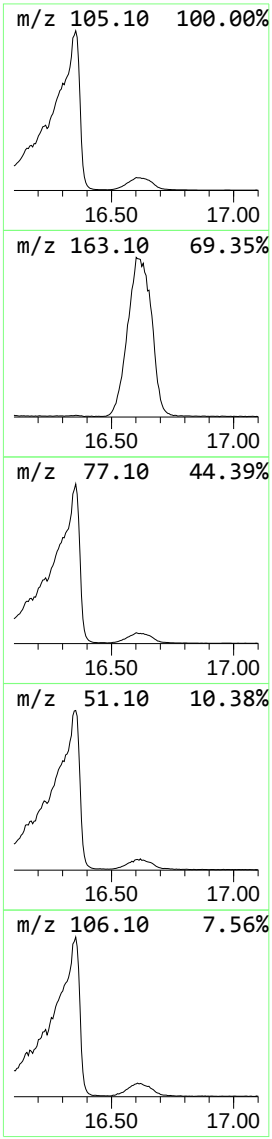
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Oxybis(propane-1,2-diyl) di... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.601	39.45 ng	1296140	Phenanthrene-d10	17.330

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzamide, N-propyl-	163	C10H13NO	010546-70-0	72
2	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	72
3	Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	53
4	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	53
5	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121721\
Data File : BM033500.D
Acq On : 17 Dec 2021 11:20
Operator : CG/JU
Sample : M5089-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

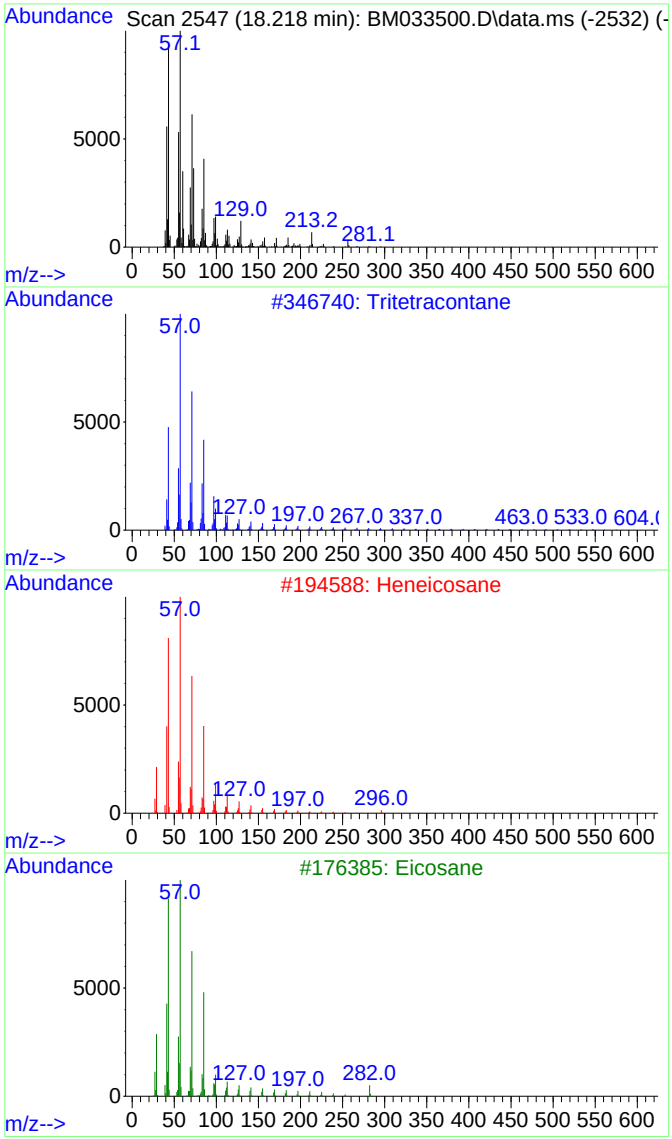
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

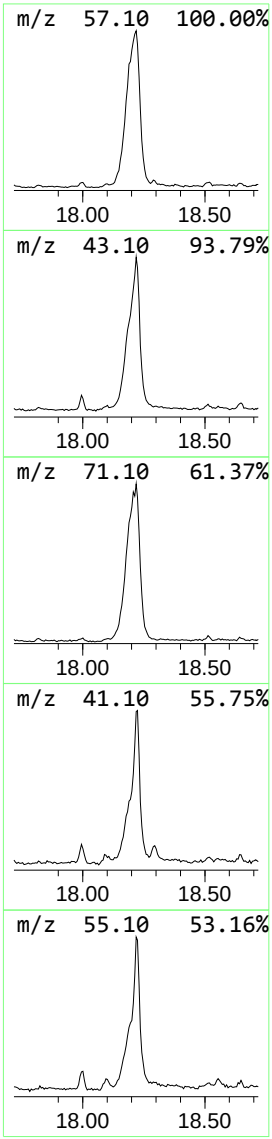
****

Peak Number 6 Tritetracontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.218	46.48 ng	1526940	Phenanthrene-d10	17.330

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tritetracontane	605	C43H88	007098-21-7	58
2	Heneicosane	296	C21H44	000629-94-7	58
3	Eicosane	282	C20H42	000112-95-8	58
4	10-Methylnonadecane	282	C20H42	056862-62-5	58
5	2-Methyltetracosane	352	C25H52	001560-78-7	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121721\
Data File : BM033500.D
Acq On : 17 Dec 2021 11:20
Operator : CG/JU
Sample : M5089-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

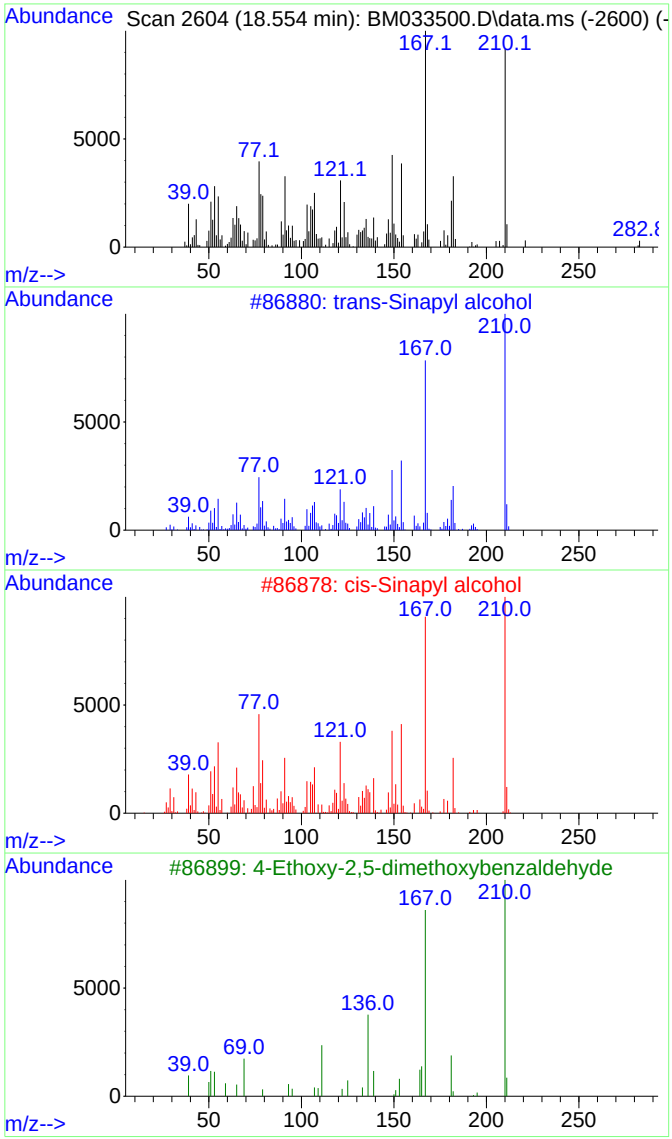
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

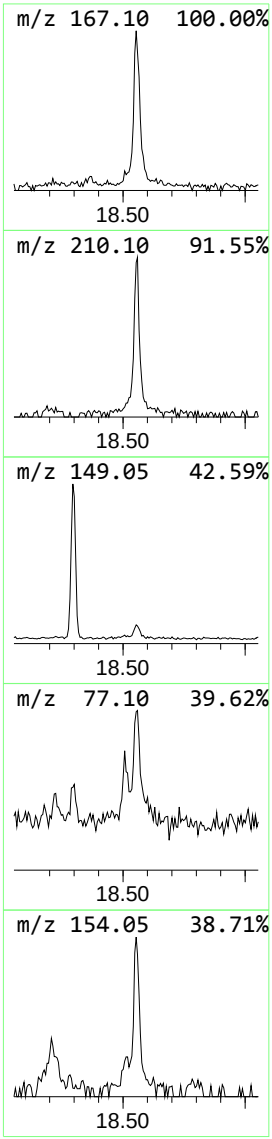
****

Peak Number 7 trans-Sinapyl alcohol Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.554	4.97 ng	163410	Phenanthrene-d10	17.330

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-Sinapyl alcohol	210	C11H14O4	020675-96-1	95
2	cis-Sinapyl alcohol	210	C11H14O4	104330-63-4	91
3	4-Ethoxy-2,5-dimethoxybenzaldehyde	210	C11H14O4	1000121-30-2	41
4	4'-(.beta.-Chloroethyl)acetophenone	182	C10H11ClO	069614-95-5	30
5	4-Ethyl-2,6-dimethoxyphenol	182	C10H14O3	014059-92-8	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121721\
Data File : BM033500.D
Acq On : 17 Dec 2021 11:20
Operator : CG/JU
Sample : M5089-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

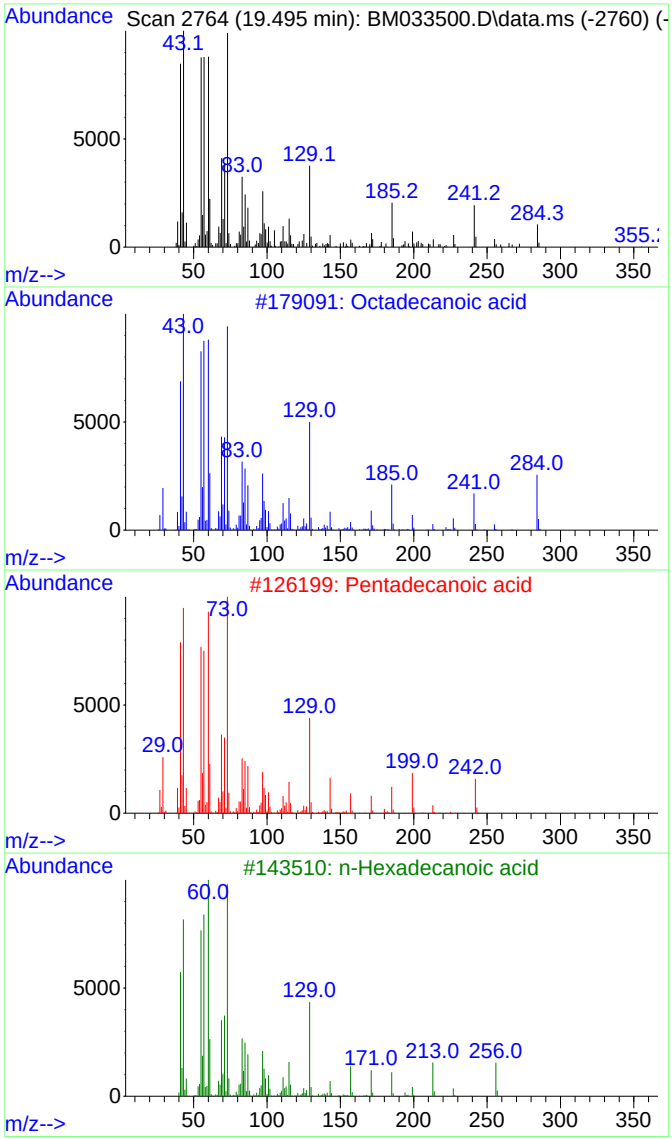
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

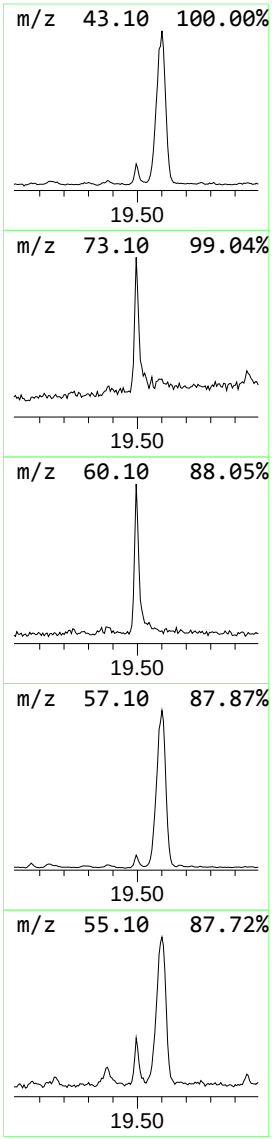
****

Peak Number 8 Octadecanoic acid Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.495	7.00 ng	209585	Chrysene-d12	21.506

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	Tridecanoic acid	214	C13H26O2	000638-53-9	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121721\
Data File : BM033500.D
Acq On : 17 Dec 2021 11:20
Operator : CG/JU
Sample : M5089-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

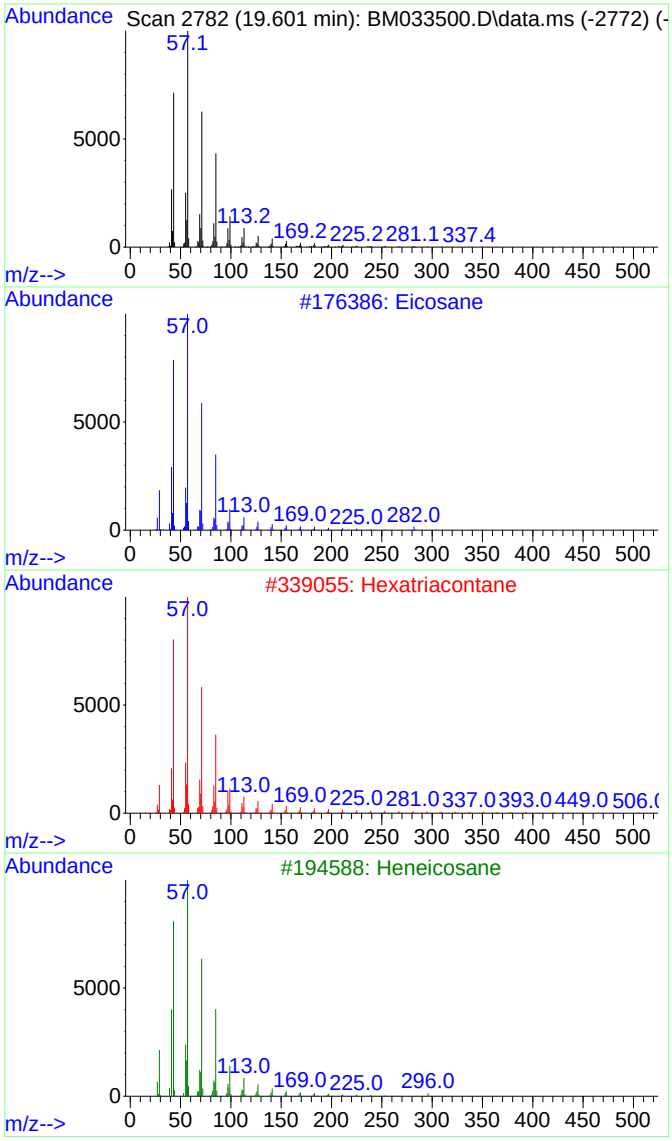
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

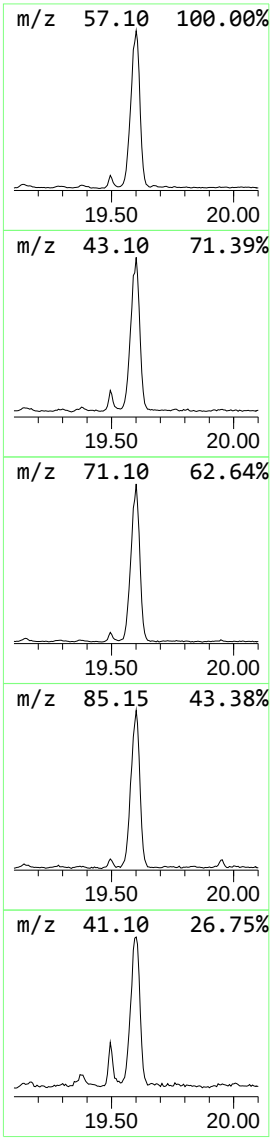
****

Peak Number 9 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.601	59.00 ng	1767120	Chrysene-d12	21.506

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Hexatriacontane	507	C36H74	000630-06-8	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





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Acq On : 17 Dec 2021 11:20
Operator : CG/JU
Sample : M5089-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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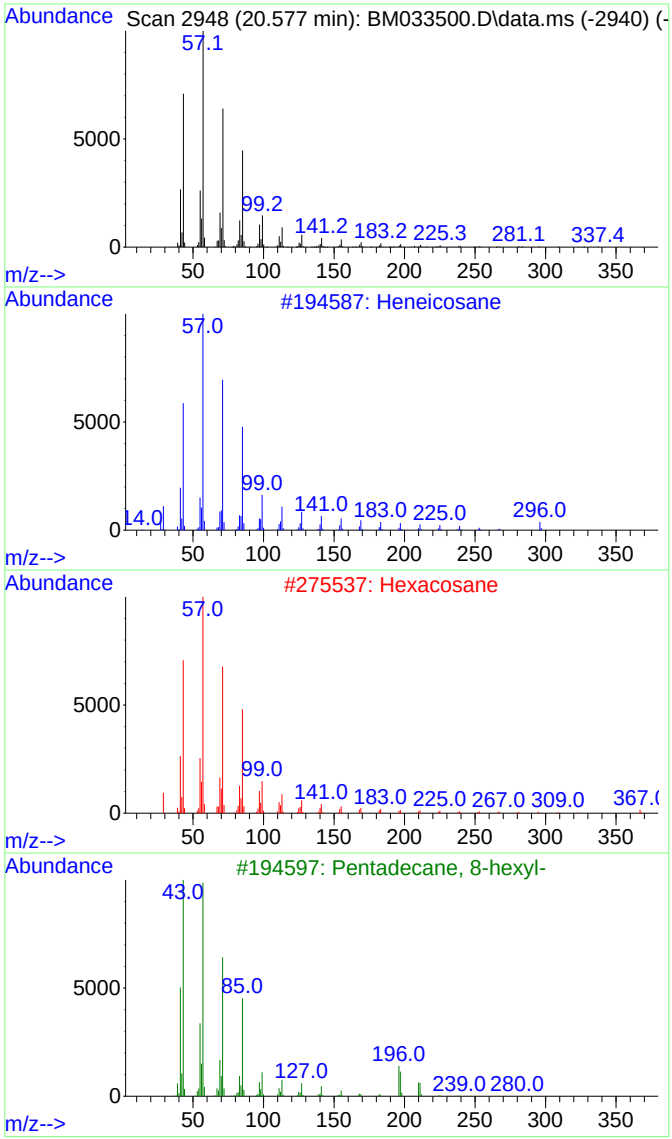
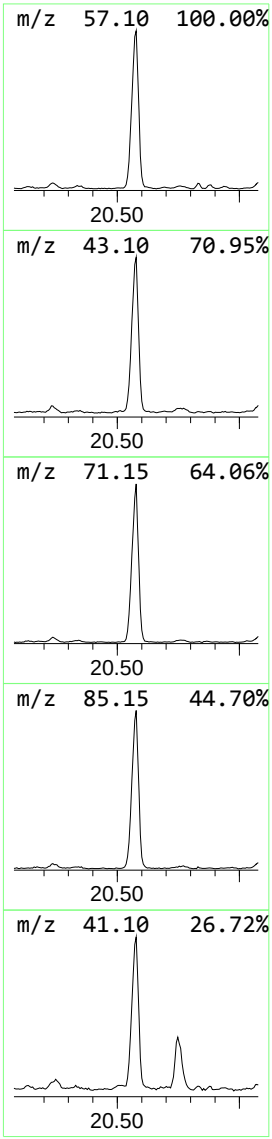
Peak Number 10 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.577	61.24 ng	1834060	Chrysene-d12	21.506

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	97
2	Hexacosane	366	C26H54	000630-01-3	94
3	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	93
4	Eicosane, 3-methyl-	296	C21H44	006418-46-8	91
5	Tetratetracontane	619	C44H90	007098-22-8	91





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Sample : M5089-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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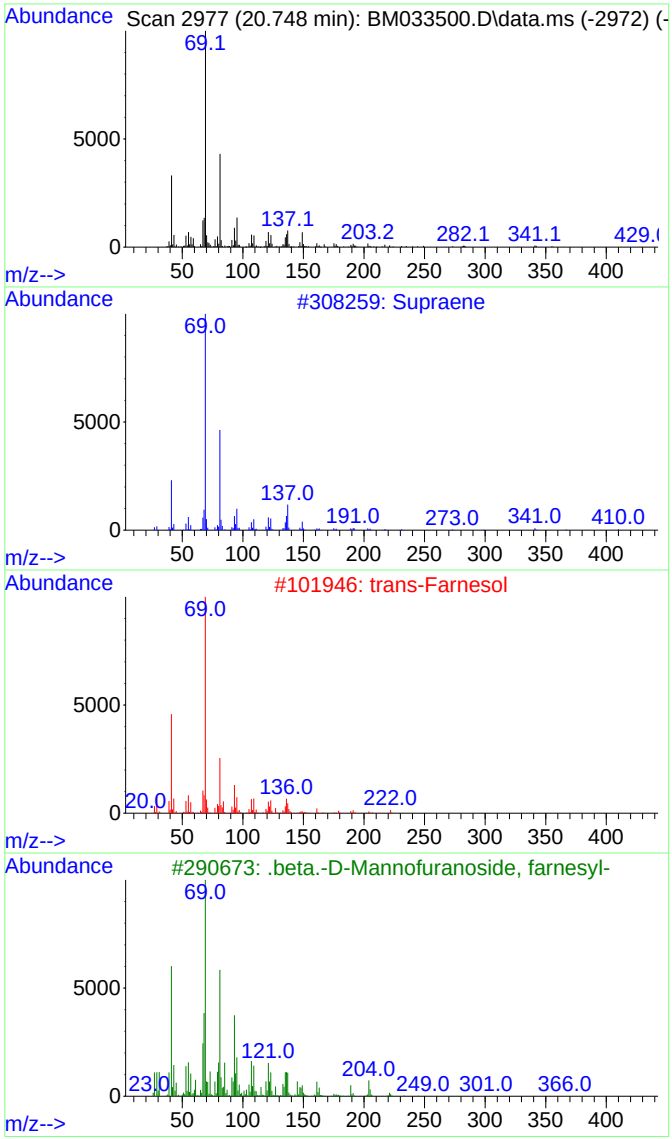
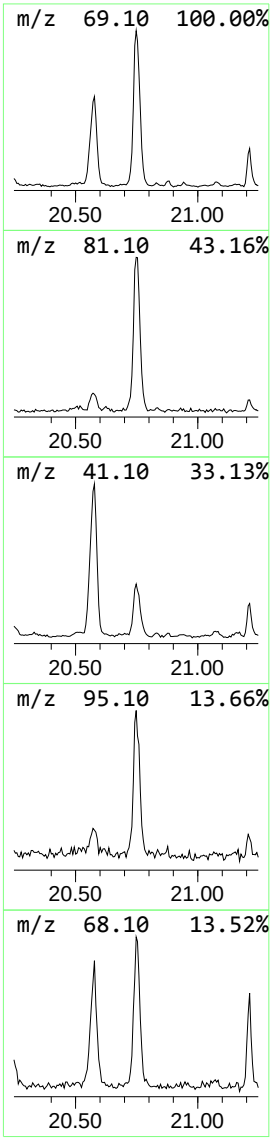
Peak Number 11 Supraene Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.748	15.58 ng	466753	Chrysene-d12	21.506

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	trans-Farnesol	222	C15H26O	000106-28-5	86
3	.beta.-D-Mannofuranoside, farnesyl-	384	C21H36O6	1000155-15-5	83
4	Squalene	410	C30H50	000111-02-4	83
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72





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Sample : M5089-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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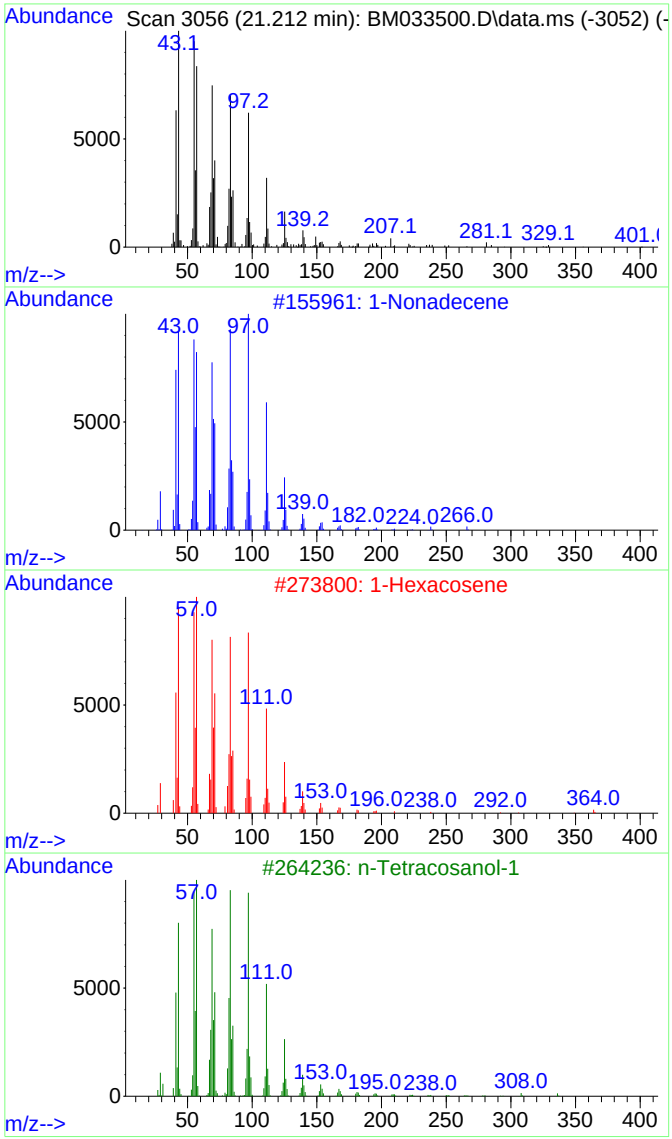
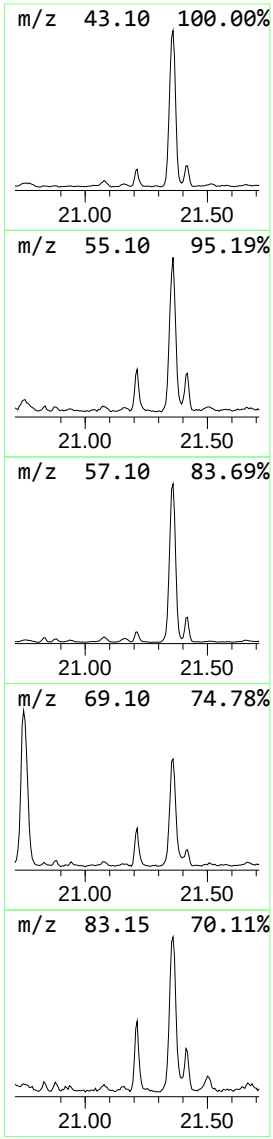
Peak Number 12 1-Nonadecene Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.212	7.69 ng	230340	Chrysene-d12	21.506

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	97
2	1-Hexacosene	364	C26H52	018835-33-1	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
5	1-Hexacosanol	382	C26H54O	000506-52-5	91





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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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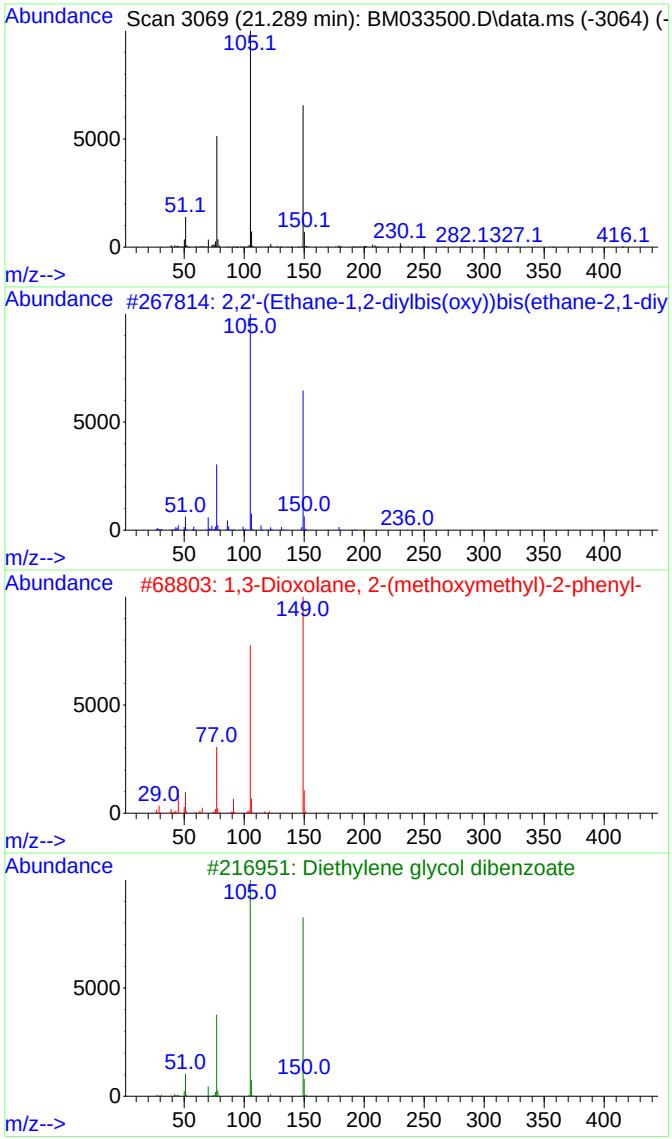
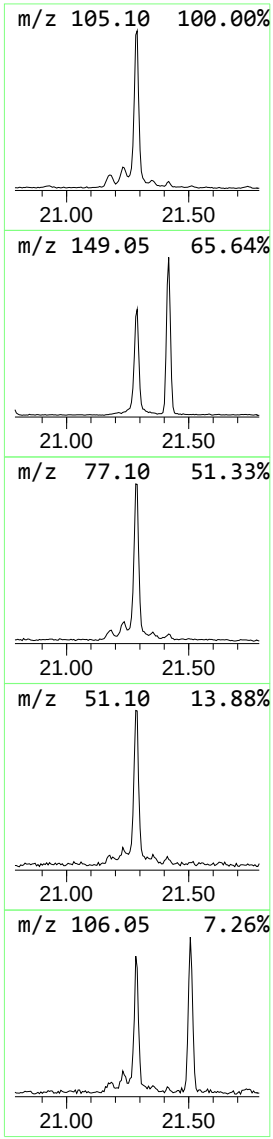
Peak Number 13 2,2'-(Ethane-1,2-diylbis(ox... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.289	12.84 ng	384545	Chrysene-d12	21.506

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	83
2	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	64
3	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	53
4	4'-Nitrobenzanilide	242	C13H10N2O3	003393-96-2	49
5	1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	49





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Sample : M5089-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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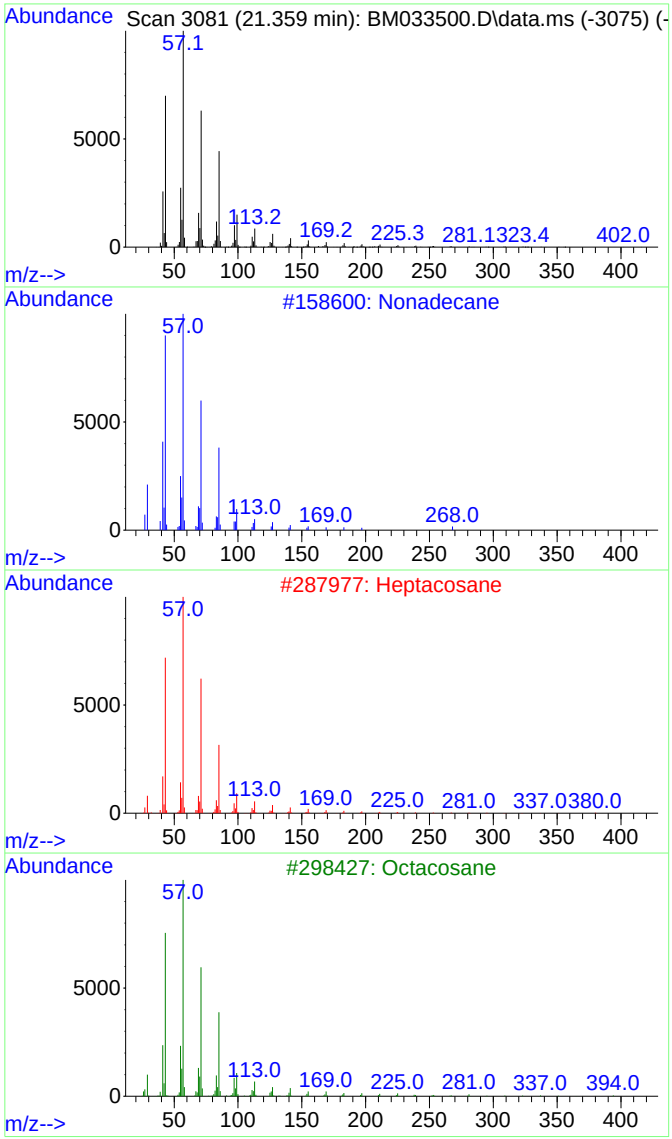
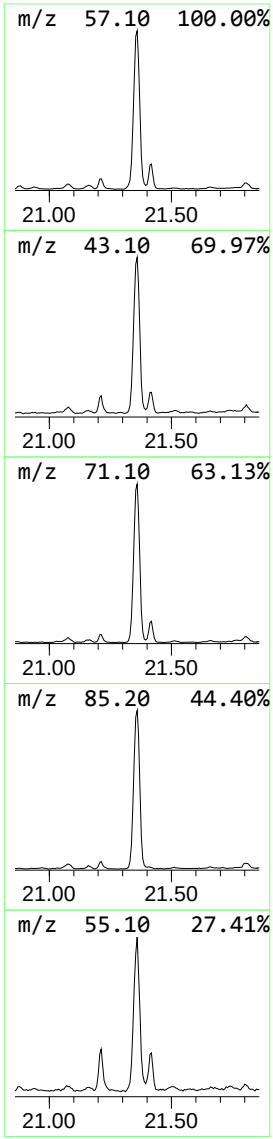
Peak Number 14 Nonadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.359	69.37 ng	2077730	Chrysene-d12	21.506

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	94
2	Heptacosane	380	C27H56	000593-49-7	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91





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Operator : CG/JU
Sample : M5089-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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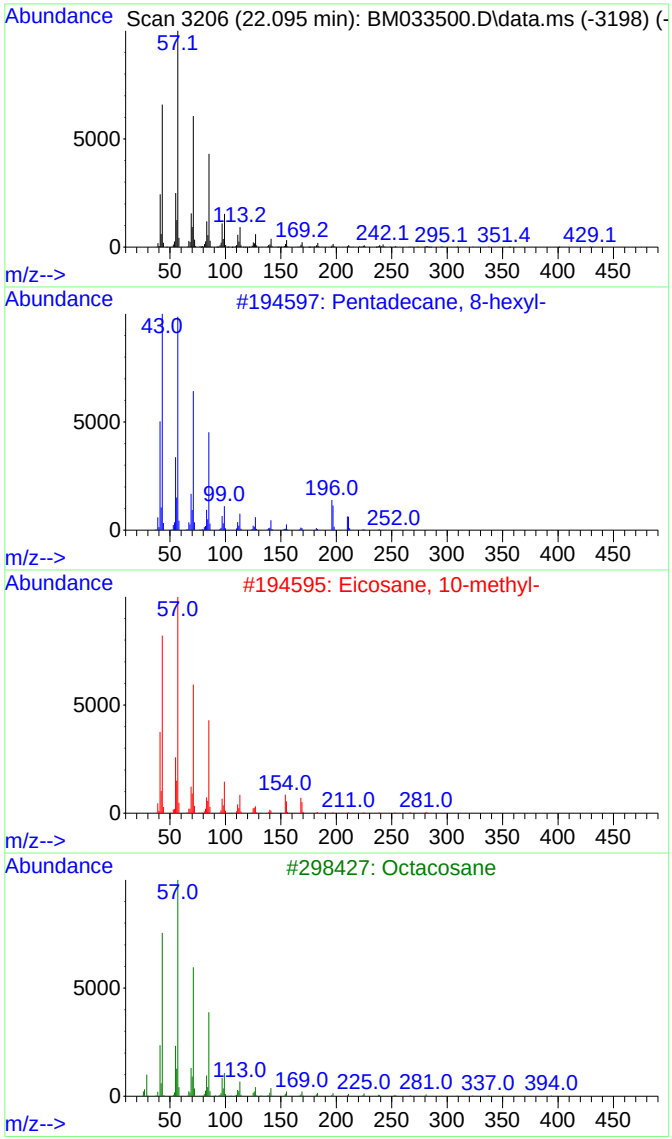
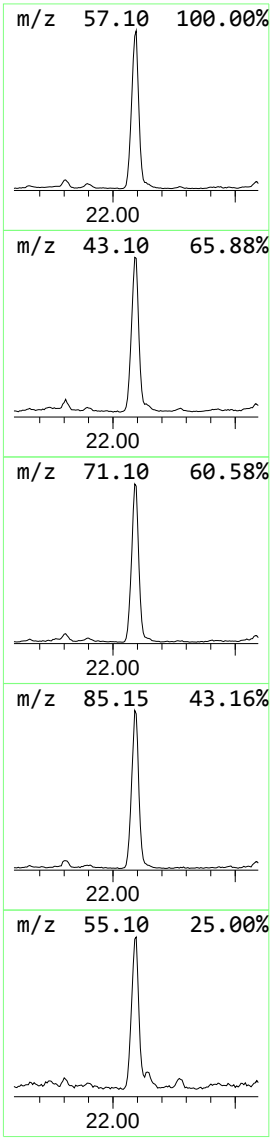
Peak Number 15 Pentadecane, 8-hexyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.095	57.30 ng	1716070	Chrysene-d12	21.506

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	94
2	Eicosane, 10-methyl-	296	C21H44	054833-23-7	94
3	Octacosane	394	C28H58	000630-02-4	91
4	Eicosane, 3-methyl-	296	C21H44	006418-46-8	91
5	Pentacosane	352	C25H52	000629-99-2	91





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Acq On : 17 Dec 2021 11:20
Operator : CG/JU
Sample : M5089-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-2

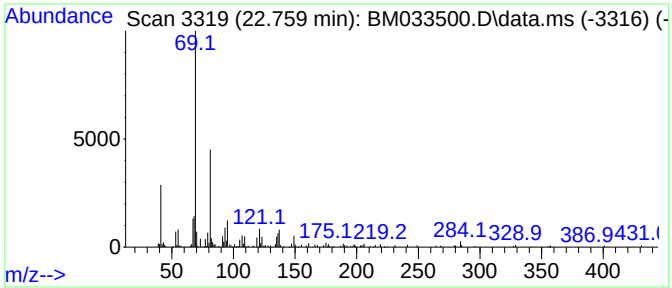
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

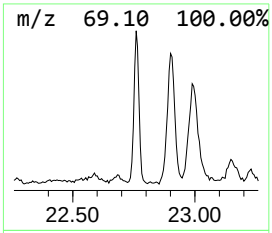
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

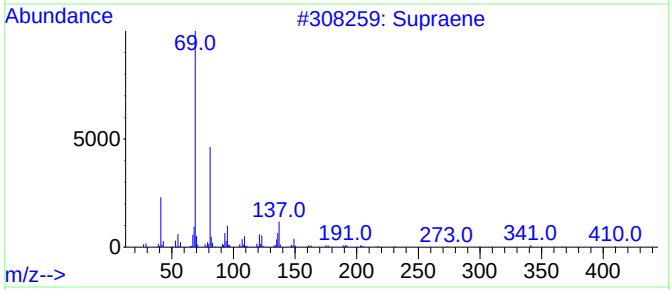
****
Peak Number 16 3,7,11-Tridecatrienenitrile... Concentration Rank 19

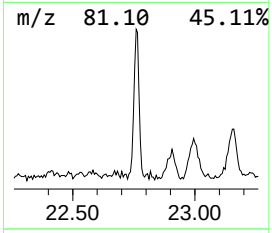
R.T.	EstConc	Area	Relative to ISTD	R.T.
22.759	6.57 ng	145447	Perylene-d12	23.924

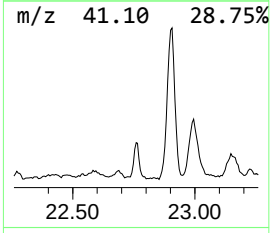
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	90
2	3,7,11-Tridecatrienenitrile, 4,8...	231	C16H25N	006006-01-5	64
3	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
5	4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	64

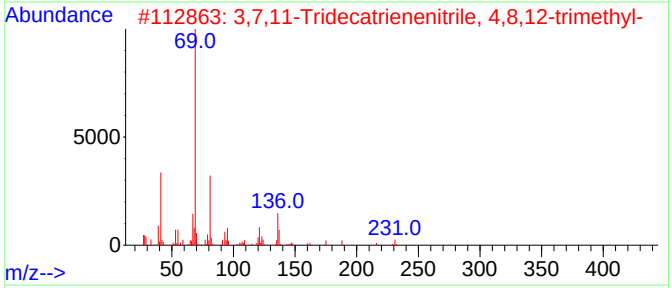


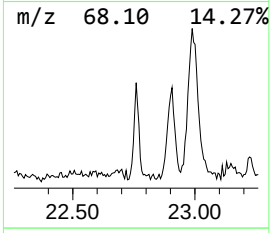


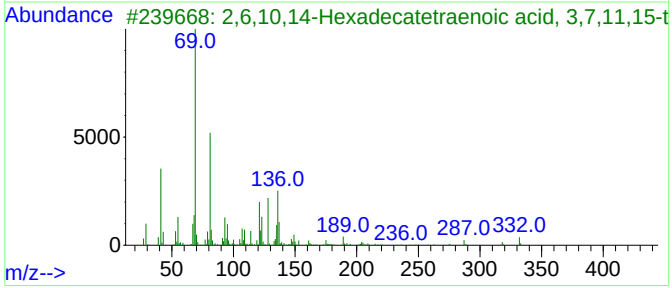


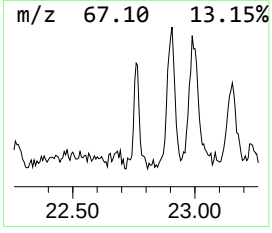












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Acq On : 17 Dec 2021 11:20
Operator : CG/JU
Sample : M5089-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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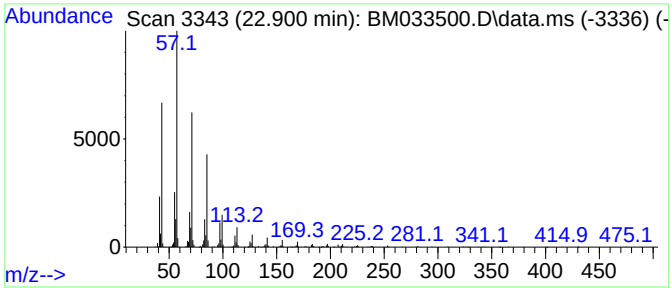
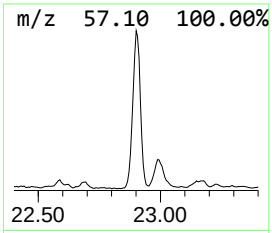
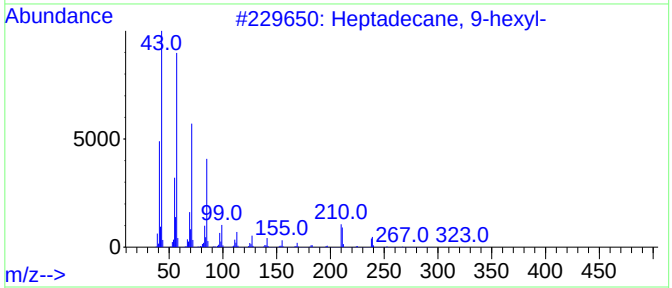
Peak Number 17 Heptadecane, 9-hexyl- Concentration Rank 4

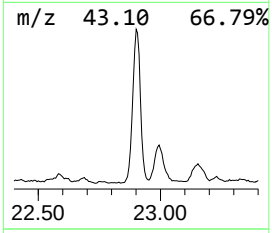
R.T.	EstConc	Area	Relative to ISTD	R.T.
22.900	68.61 ng	1519970	Perylene-d12	23.924

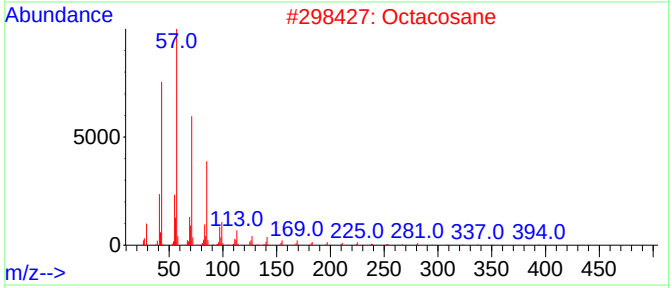
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	94
2	Octacosane	394	C28H58	000630-02-4	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Pentacosane	352	C25H52	000629-99-2	91
5	Heptacosane	380	C27H56	000593-49-7	91

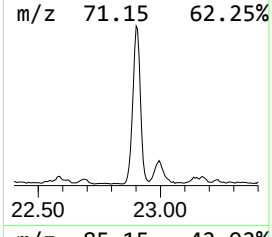


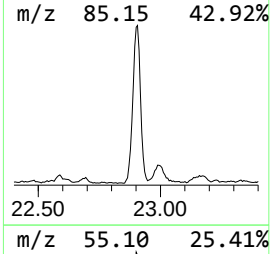


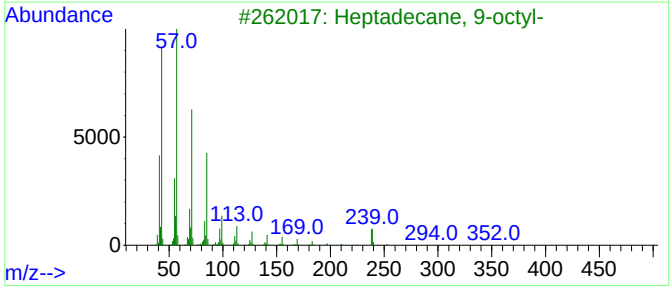


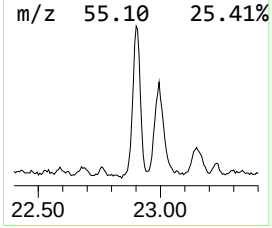












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Acq On : 17 Dec 2021 11:20
Operator : CG/JU
Sample : M5089-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-2

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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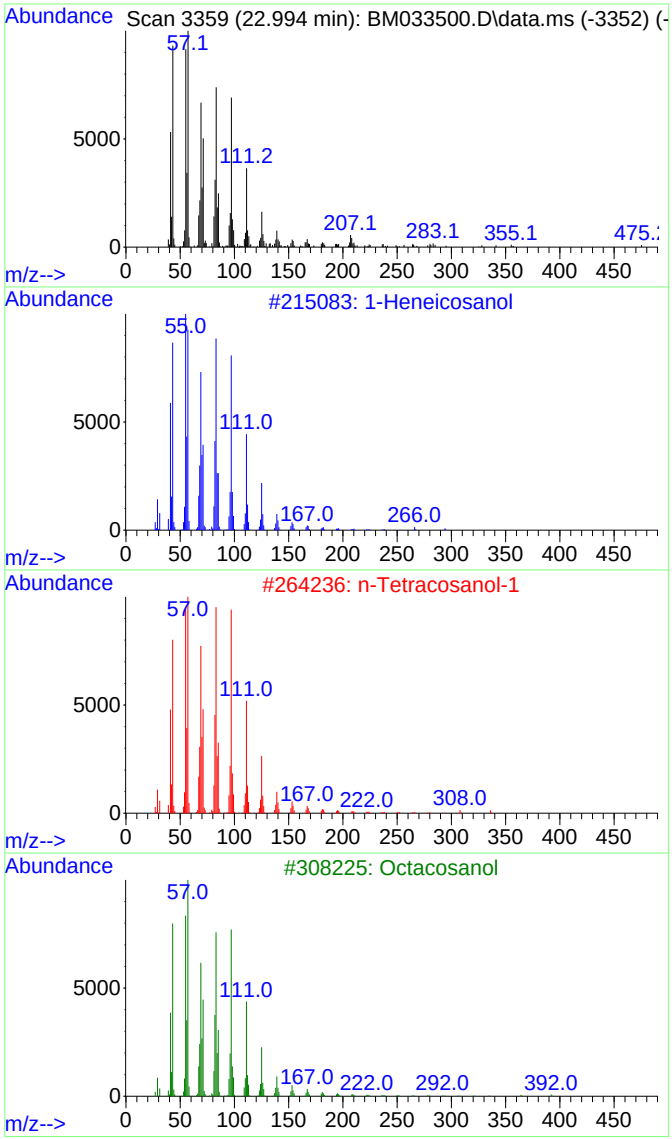
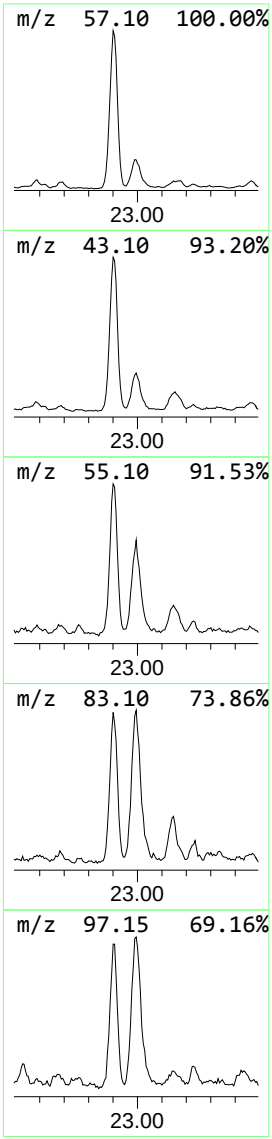
Peak Number 18 1-Heneicosanol Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.994	28.95 ng	641408	Perylene-d12	23.924

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
3	Octacosanol	410	C28H58O	000557-61-9	93
4	1-Hexacosene	364	C26H52	018835-33-1	93
5	Behenic alcohol	326	C22H46O	000661-19-8	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121721\
Data File : BM033500.D
Acq On : 17 Dec 2021 11:20
Operator : CG/JU
Sample : M5089-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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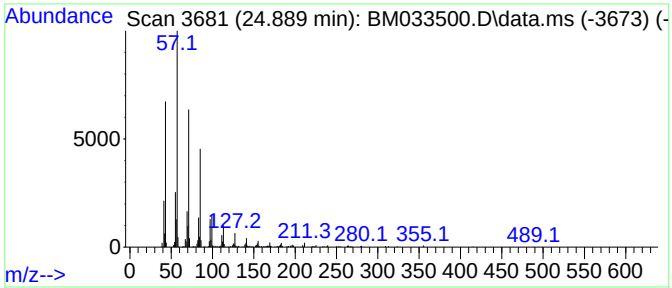
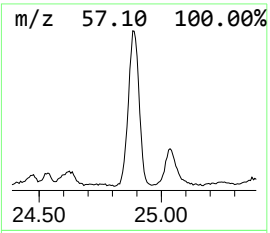
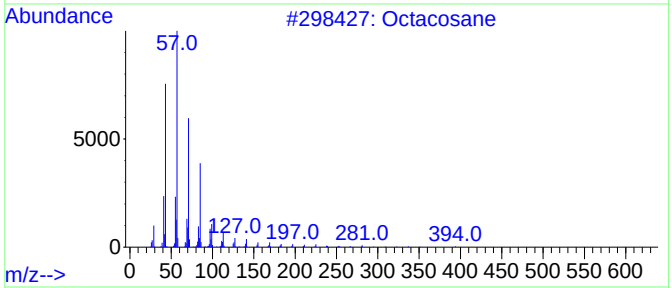
Peak Number 19 Octacosane Concentration Rank 9

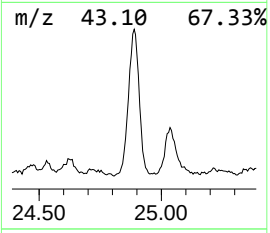
R.T.	EstConc	Area	Relative to ISTD	R.T.
24.889	41.67 ng	923183	Perylene-d12	23.924

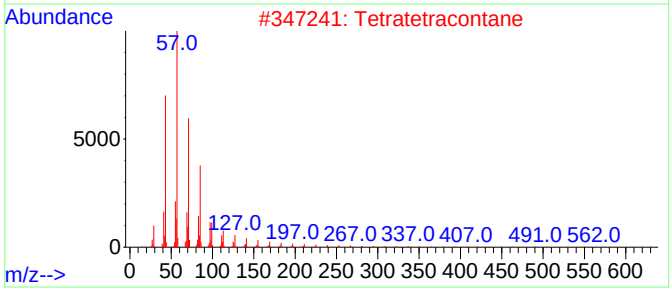
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Tetratetracontane	619	C44H90	007098-22-8	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91

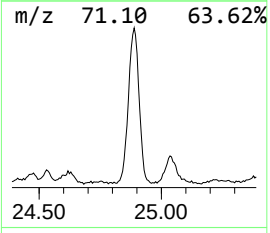


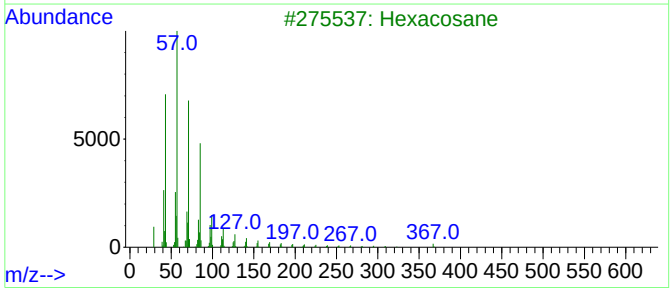


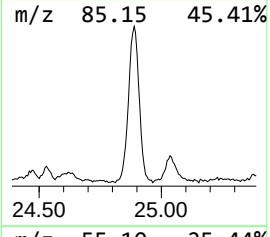


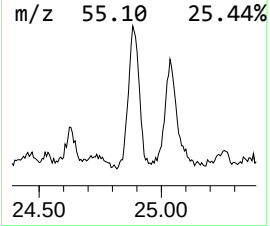












Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121721\
Data File : BM033500.D
Acq On : 17 Dec 2021 11:20
Operator : CG/JU
Sample : M5089-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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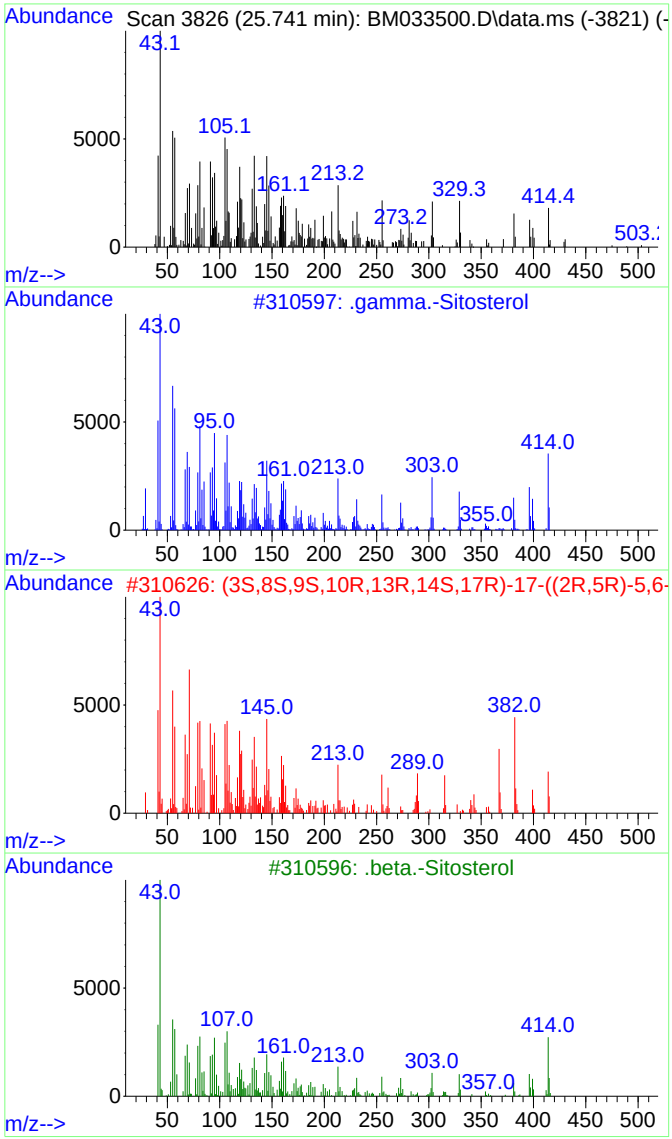
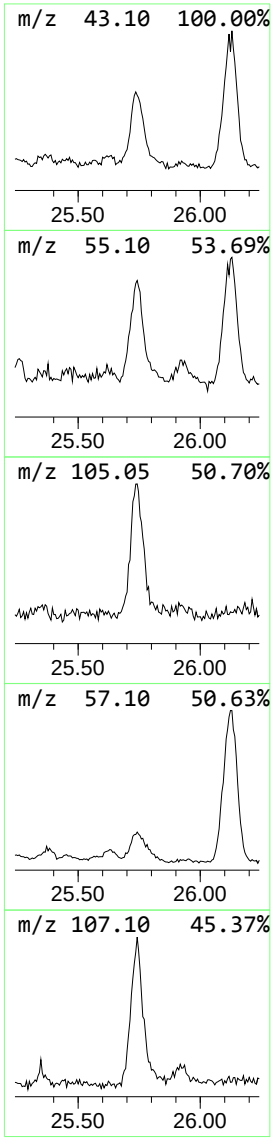
Peak Number 20 .gamma.-Sitosterol Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.741	27.71 ng	613878	Perylene-d12	23.924

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Sitosterol	414	C29H50O	000083-47-6	90
2	(3S,8S,9S,10R,13R,14S,17R)-17-((...	414	C29H50O	029365-29-5	78
3	.beta.-Sitosterol	414	C29H50O	000083-46-5	64
4	(3S,8S,9S,10R,13R,14S,17R)-17-((...	428	C30H52O	020194-50-7	43
5	5-Cholesten-3.beta.-acetoxy-24-t...	460	C29H48O2S	1000253-09-1	37





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121721\
Data File : BM033500.D
Acq On : 17 Dec 2021 11:20
Operator : CG/JU
Sample : M5089-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.037	29.5	ng	356428	1	7.931	241940	20.0
Benzamide, N-pr...	14.889	34.9	ng	814393	3	14.583	467029	20.0
Morpholine, 4-p...	15.736	270.2	ng	6308920	3	14.583	467029	20.0
Diethylene glyc...	16.354	359.5	ng	11810800	4	17.330	657096	20.0
Oxybis(propane-...	16.601	39.5	ng	1296140	4	17.330	657096	20.0
Tritetracontane	18.218	46.5	ng	1526940	4	17.330	657096	20.0
trans-Sinapyl a...	18.554	5.0	ng	163410	4	17.330	657096	20.0
Octadecanoic acid	19.495	7.0	ng	209585	5	21.506	598998	20.0
Eicosane	19.601	59.0	ng	1767120	5	21.506	598998	20.0
Heneicosane	20.577	61.2	ng	1834060	5	21.506	598998	20.0
Supraene	20.748	15.6	ng	466753	5	21.506	598998	20.0
1-Nonadecene	21.212	7.7	ng	230340	5	21.506	598998	20.0
2,2'-(Ethane-1,...	21.289	12.8	ng	384545	5	21.506	598998	20.0
Nonadecane	21.359	69.4	ng	2077730	5	21.506	598998	20.0
Pentadecane, 8-...	22.095	57.3	ng	1716070	5	21.506	598998	20.0
3,7,11-Tridecat...	22.759	6.6	ng	145447	6	23.924	443059	20.0
Heptadecane, 9-...	22.900	68.6	ng	1519970	6	23.924	443059	20.0
1-Heneicosanol	22.994	28.9	ng	641408	6	23.924	443059	20.0
Octacosane	24.889	41.7	ng	923183	6	23.924	443059	20.0
.gamma.-Sitosterol	25.741	27.7	ng	613878	6	23.924	443059	20.0