LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121721\
Data File : BM033501.D
Acq On : 17 Dec 2021 11:56
Operator : CG/JU
Sample : M5089-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-3

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: BM033501.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.431	198	203	209	rBV	36144	52576	1.58%	0.209%
2	5.037	300	306	315	rBV	433048	626623	18.88%	2.495%
3	5.502	378	385	396	rBV	1209758	1751527	52.76%	6.975%
4	6.119	484	490	497	rBV	36101	50207	1.51%	0.200%
5	7.107	645	658	671	rBV	1192387	1986907	59.85%	7.912%
6	7.543	727	732	737	rBV	28535	39857	1.20%	0.159%
7	7.931	794	798	805	rVB	206990	338844	10.21%	1.349%
8	9.107	990	998	1004	rBV	768796	1304772	39.30%	5.196%
9	9.154	1004	1006	1012	rVB	51787	66275	2.00%	0.264%
10	10.531	1234	1240	1254	rBV	52577	102777	3.10%	0.409%
11	10.748	1266	1277	1282	rBV	278169	504250	15.19%	2.008%
12	10.795	1282	1285	1291	rVB	39556	62046	1.87%	0.247%
13	12.407	1552	1559	1569	rBV	103477	168848	5.09%	0.672%
14	12.625	1587	1596	1602	rVB	89333	145852	4.39%	0.581%
15	13.207	1688	1695	1703	rBV	1907473	2733986	82.35%	10.887%
16	13.419	1723	1731	1737	rBV	50115	87844	2.65%	0.350%
17	13.901	1807	1813	1819	rBV4	26164	53395	1.61%	0.213%
18	14.225	1864	1868	1875	rBV2	28637	42723	1.29%	0.170%
19	14.583	1919	1929	1934	rBV	427565	664953	20.03%	2.648%
20	14.648	1934	1940	1948	rVB	254148	398276	12.00%	1.586%
21	14.977	1991	1996	2006	rBV	158864	245555	7.40%	0.978%
22	15.630	2101	2107	2116	rVB	180213	267505	8.06%	1.065%
23	15.924	2152	2157	2164	rVB2	26339	47278	1.42%	0.188%
24	16.071	2176	2182	2188	rBV	1431275	2099383	63.24%	8.360%
25	16.307	2215	2222	2227	rBV6	22937	48129	1.45%	0.192%
26	16.630	2268	2277	2282	rBV5	24981	60909	1.83%	0.243%
27	17.148	2360	2365	2373	rVB	47749	90611	2.73%	0.361%
28	17.242	2378	2381	2385	rVB	41484	50307	1.52%	0.200%
29	17.330	2390	2396	2399	rBV	512346	739571	22.28%	2.945%
30	17.371	2399	2403	2409	rVB	599625	847638	25.53%	3.375%
31	17.460	2414	2418	2424	rVV	106356	156833	4.72%	0.625%
32	17.613	2440	2444	2448	rBV	41011	60317	1.82%	0.240%
33	17.736	2462	2465	2472	rVB	69520	103561	3.12%	0.412%
34	17.995	2506	2509	2513	rVB2	48892	59117	1.78%	0.235%
35	18.218	2542	2547	2551	rBV2	177210	293071	8.83%	1.167%
36	18.254	2551	2553	2557	rVV	81744	101612	3.06%	0.405%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121721\
Data File : BM033501.D
Acq On : 17 Dec 2021 11:56
Operator : CG/JU
Sample : M5089-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-3

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

37	18.295	2557	2560	2564	rVB	52145	57164	1.72%	0.228%
38	18.401	2574	2578	2583	rBV3	108331	174189	5.25%	0.694%
39	18.512	2594	2597	2601	rBV5	31637	44189	1.33%	0.176%
40	18.707	2627	2630	2634	rVB	53263	65501	1.97%	0.261%
41	19.383	2740	2745	2751	rBV	963469	1322551	39.84%	5.267%
42	19.495	2761	2764	2768	rBV2	82043	107196	3.23%	0.427%
43	19.718	2798	2802	2803	rBV2	163037	188156	5.67%	0.749%
44	19.748	2803	2807	2816	rVB	675934	956499	28.81%	3.809%
45	19.954	2836	2842	2847	rVB	2645336	3319812	100.00%	13.220%
46	21.212	3053	3056	3065	rVB3	224137	316877	9.55%	1.262%
47	21.418	3087	3091	3096	rVB	641133	692102	20.85%	2.756%
48	21.506	3100	3106	3110	rBV2	446484	854876	25.75%	3.404%
49	21.548	3110	3113	3118	rVB	176848	223262	6.73%	0.889%
50	23.930	3513	3518	3524	rVB2	177456	335893	10.12%	1.338%

Sum of corrected areas: 25112202

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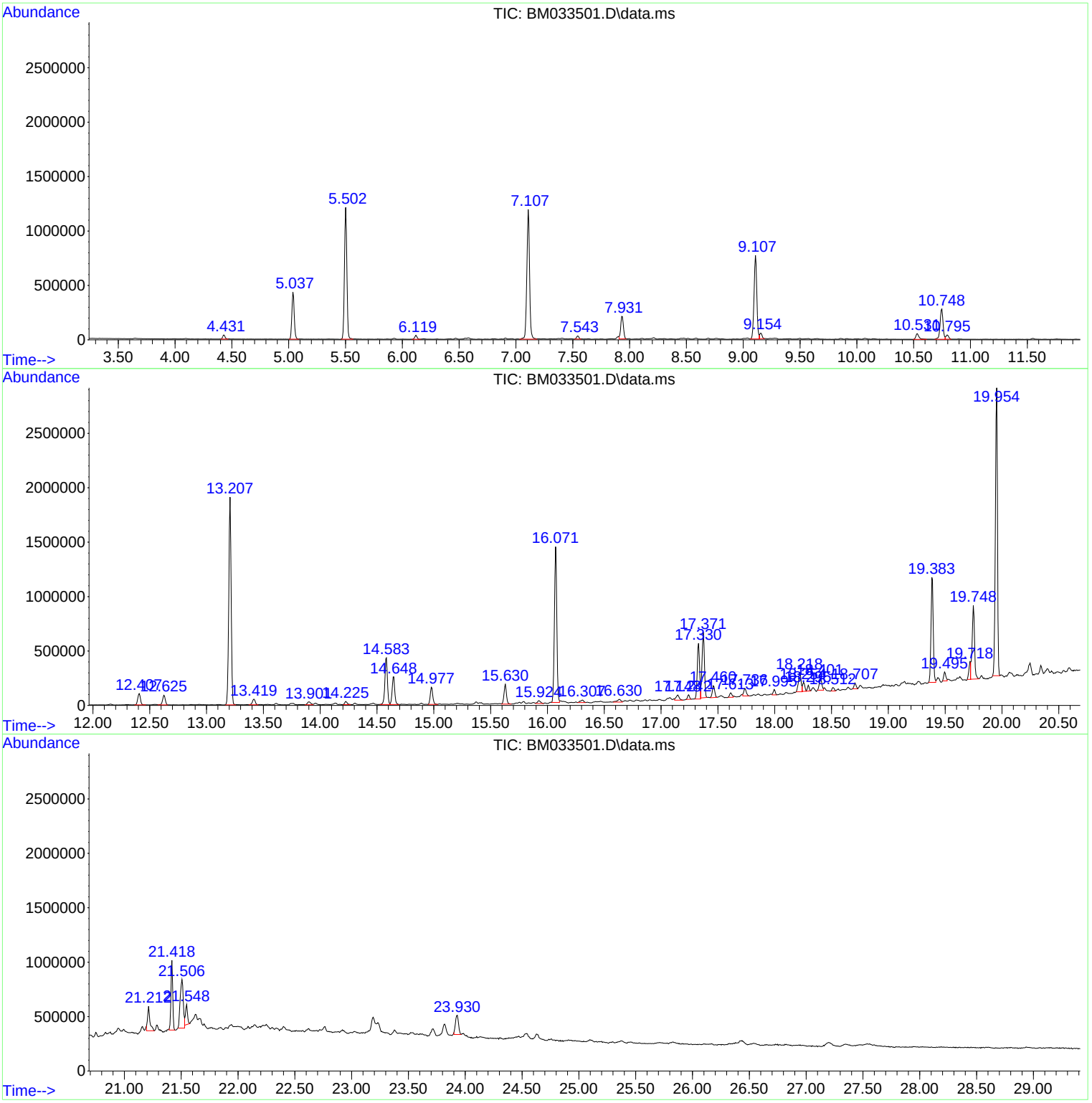
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-3

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 : BM033501.D
Acq On : 17 Dec 2021 11:56
Operator : CG/JU
Sample : M5089-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

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

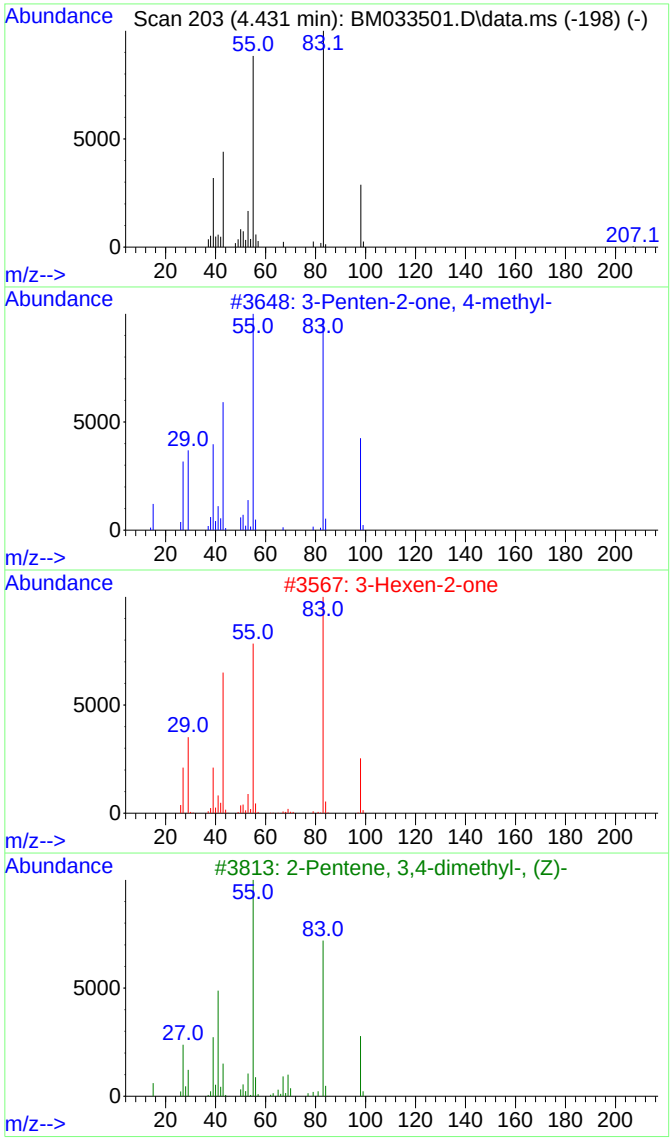
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

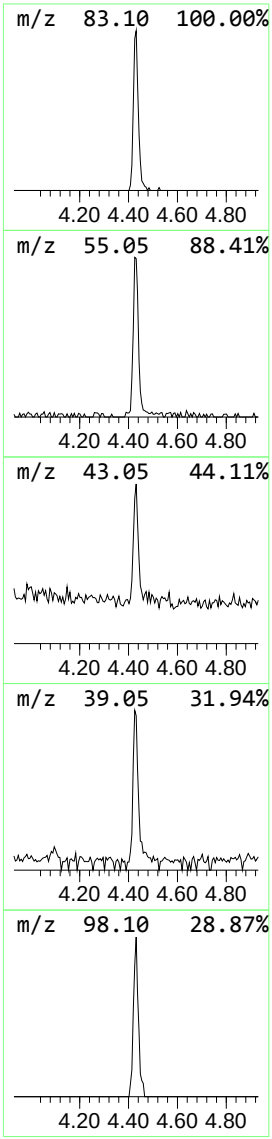
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.431	3.10 ng	52576	1,4-Dichlorobenzene-d4	7.937

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	87
2	3-Hexen-2-one	98	C6H10O	000763-93-9	86
3	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	80
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
5	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121721\
Data File : BM033501.D
Acq On : 17 Dec 2021 11:56
Operator : CG/JU
Sample : M5089-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

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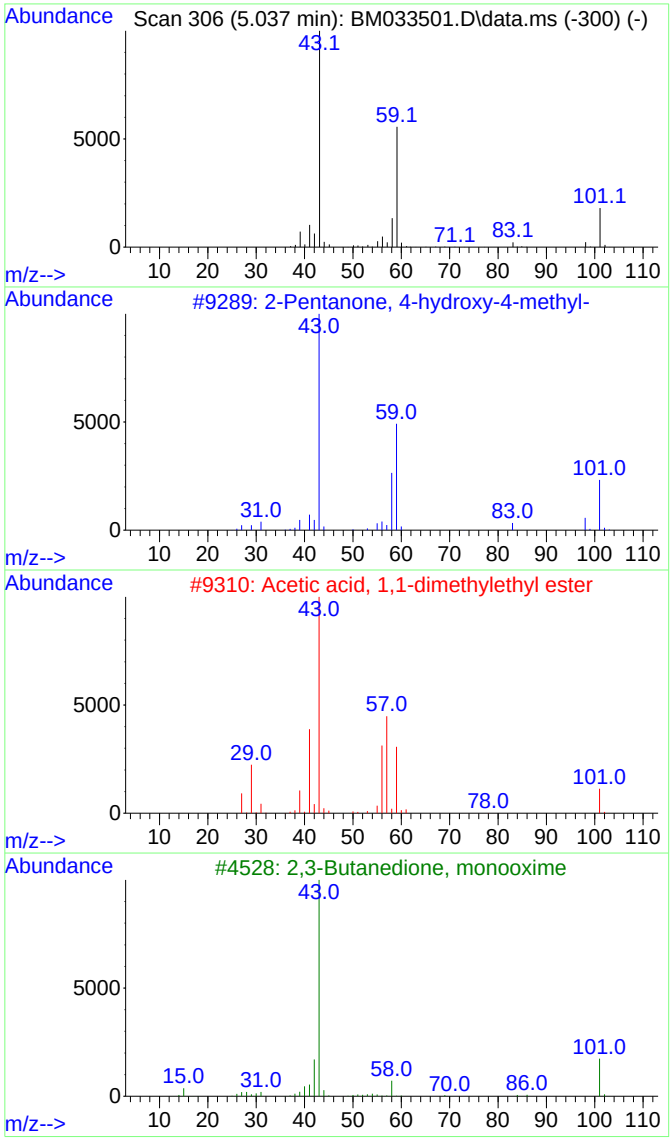
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

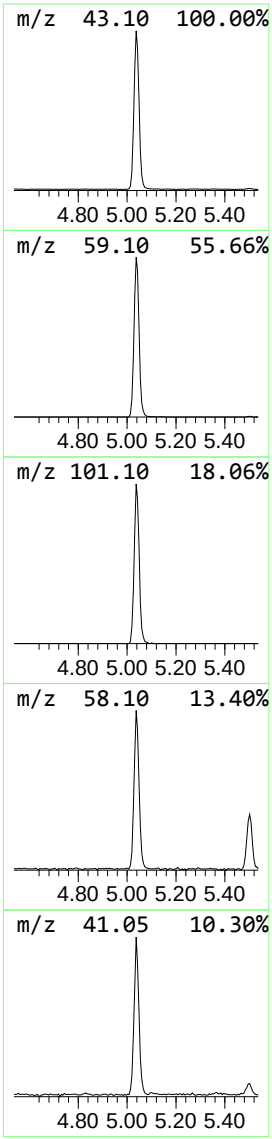
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.037	36.99 ng	626623	1,4-Dichlorobenzene-d4	7.937

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Data File : BM033501.D
Acq On : 17 Dec 2021 11:56
Operator : CG/JU
Sample : M5089-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-3

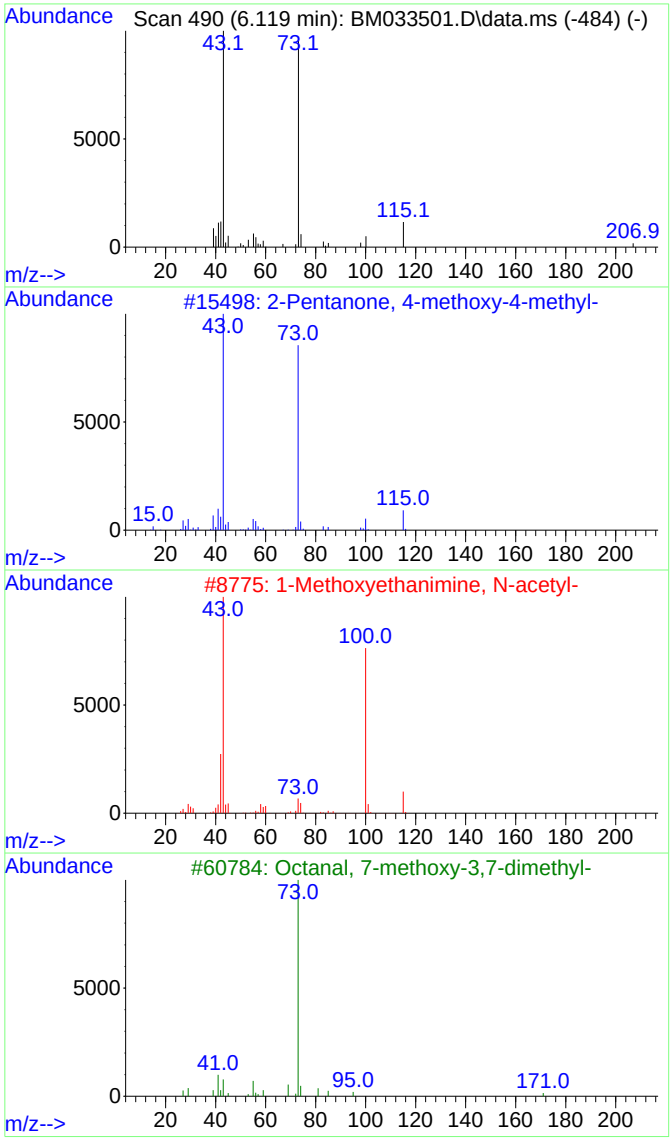
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

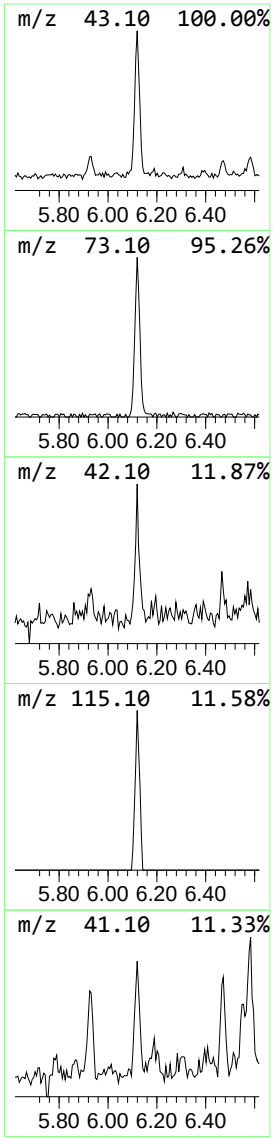
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.119	2.96 ng	50207	1,4-Dichlorobenzene-d4	7.937

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	43
3	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
4	7-Methoxy-3,7-dimethyloctan-2-ol...	188	C11H24O2	1000511-09-7	12
5	Butane, 2,3-dimethoxy-2-methyl-	132	C7H16O2	074421-00-4	12





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Acq On : 17 Dec 2021 11:56
Operator : CG/JU
Sample : M5089-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

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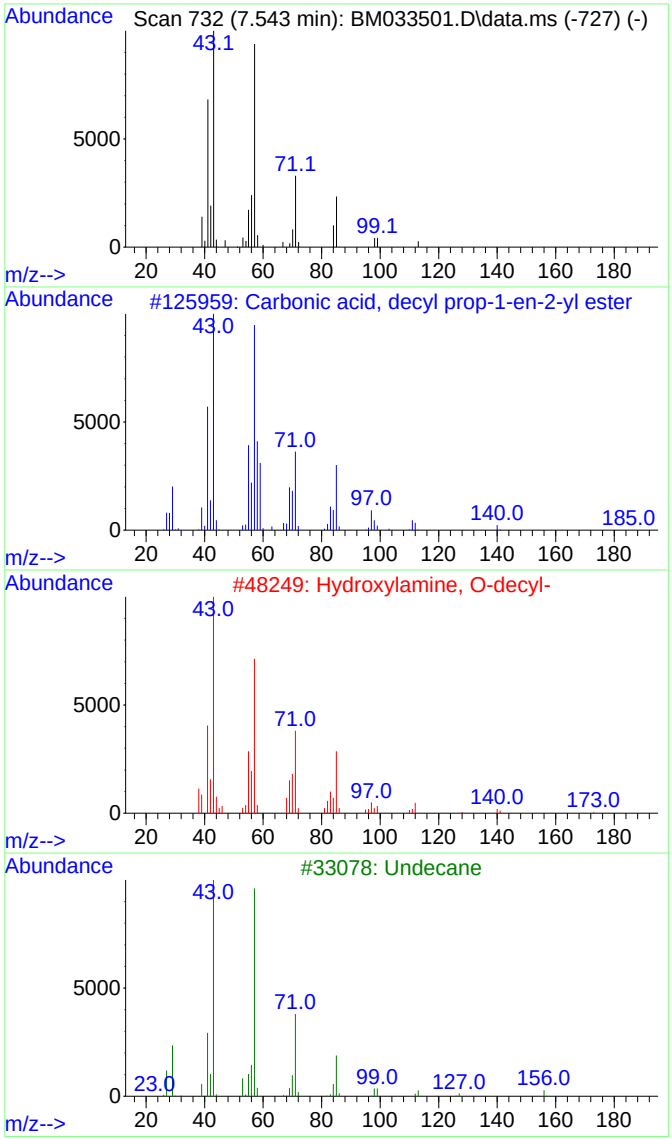
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

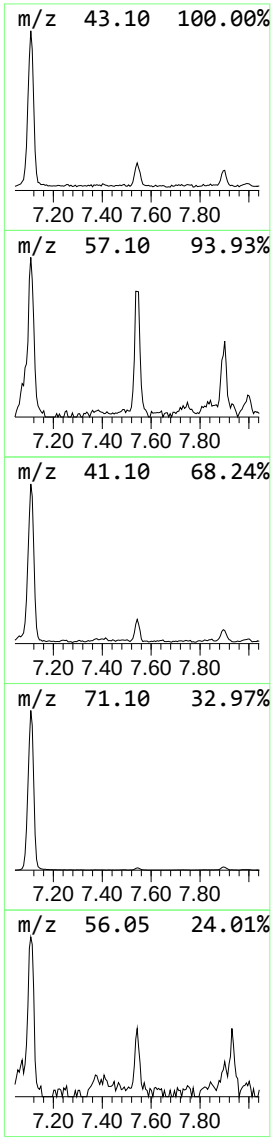
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Carbonic acid, decyl prop-1... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.543	2.35 ng	39857	1,4-Dichlorobenzene-d4	7.937

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, decyl prop-1-en-2...	242	C14H26O3	1000382-90-5	83
2	Hydroxylamine, O-decyl-	173	C10H23NO	029812-79-1	72
3	Undecane	156	C11H24	001120-21-4	64
4	Octane, 2,7-dimethyl-	142	C10H22	001072-16-8	59
5	Hexane, 2,2,3,3-tetramethyl-	142	C10H22	013475-81-5	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121721\
Data File : BM033501.D
Acq On : 17 Dec 2021 11:56
Operator : CG/JU
Sample : M5089-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-3

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

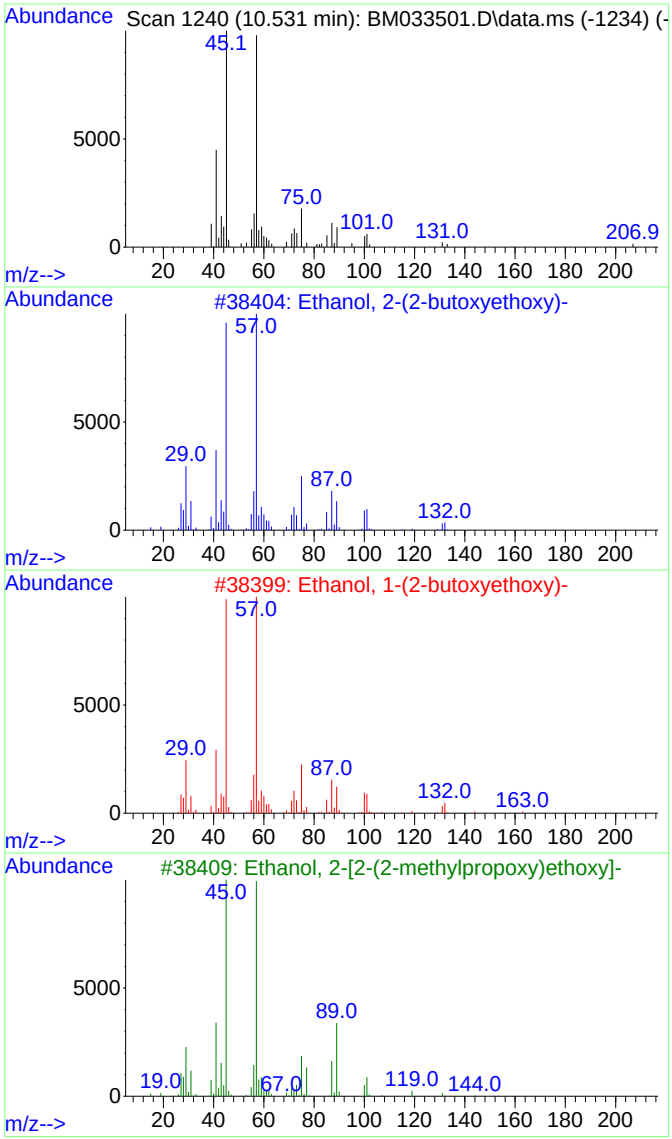
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

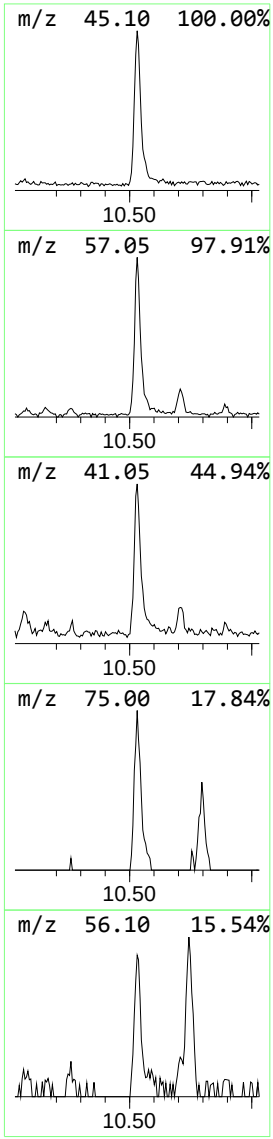
****

Peak Number 5 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.531	4.08 ng	102777	Naphthalene-d8	10.748

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	78
4	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
5	Acetaldehyde, di-sec-butyl acetal	174	C10H22O2	005314-41-0	53





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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-3

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

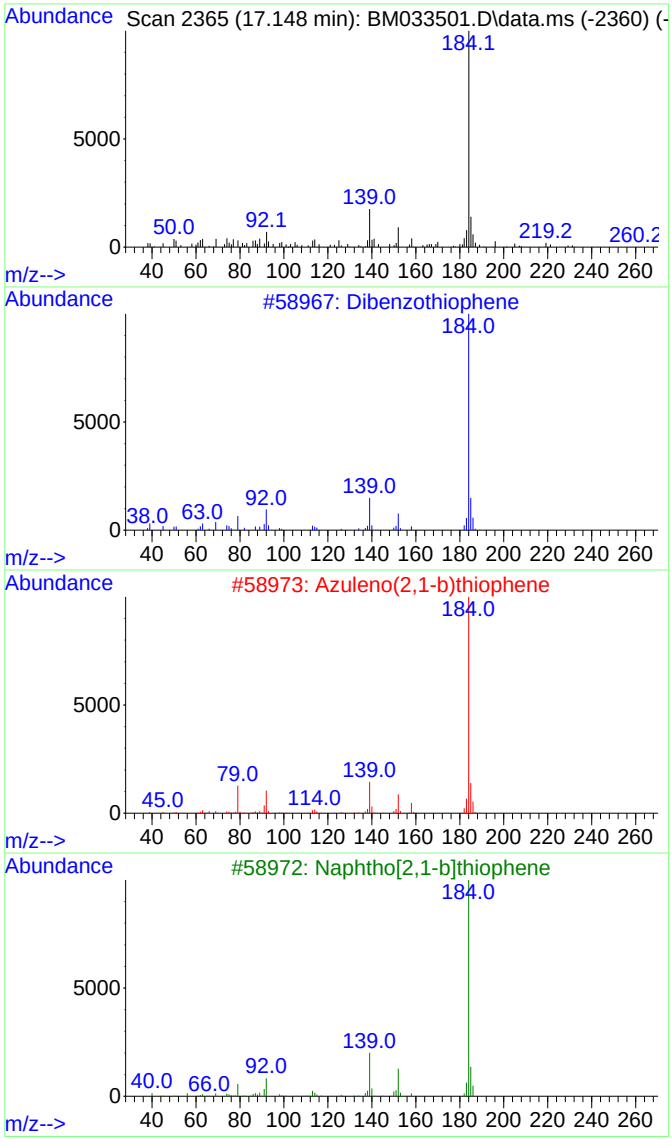
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

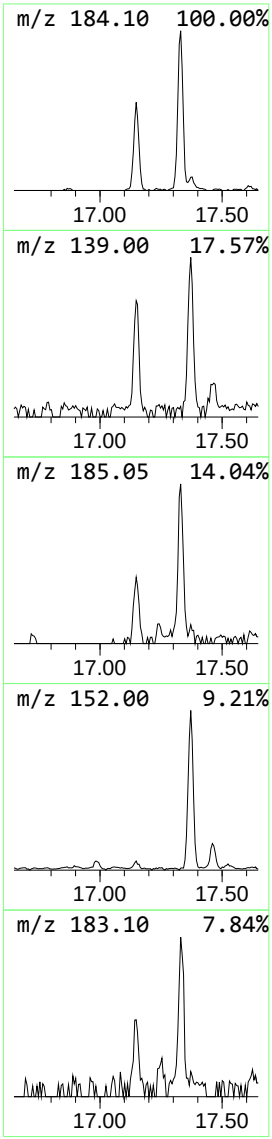
****

Peak Number 6 Dibenzothiophene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.148	2.45 ng	90611	Phenanthrene-d10	17.330

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzothiophene	184	C12H8S	000132-65-0	91
2	Azuleno(2,1-b)thiophene	184	C12H8S	000248-13-5	91
3	Naphtho[2,1-b]thiophene	184	C12H8S	000233-02-3	90
4	Naphtho[2,3-b]thiophene	184	C12H8S	000268-77-9	87
5	Naphtho[1,2-b]thiophene	184	C12H8S	000234-41-3	87





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Sample : M5089-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

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

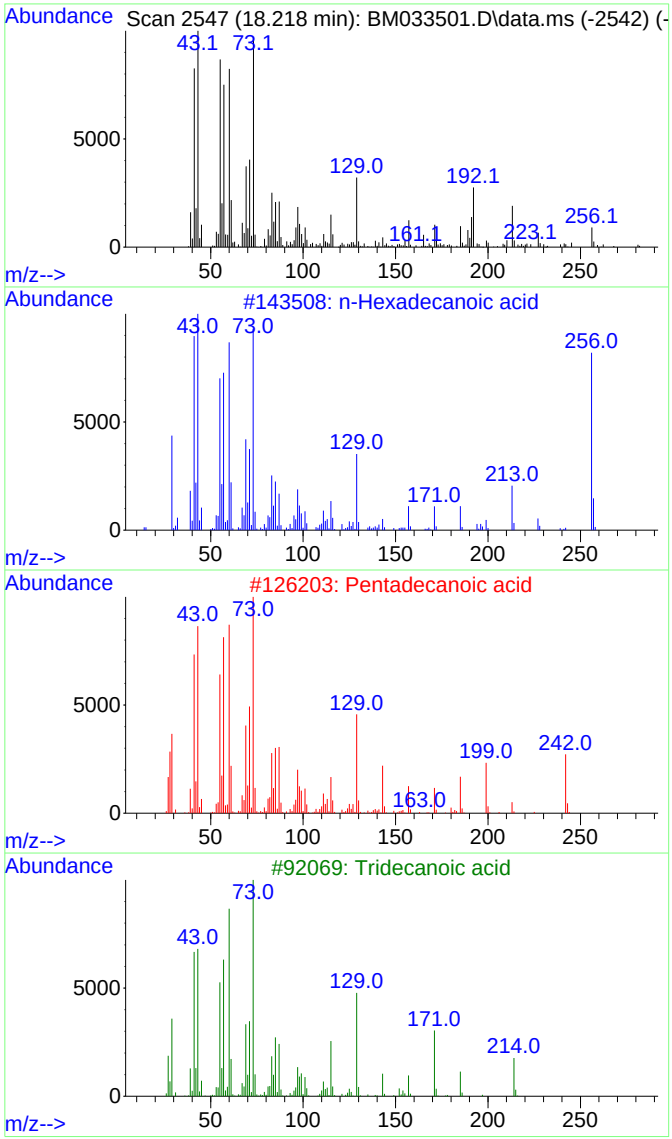
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

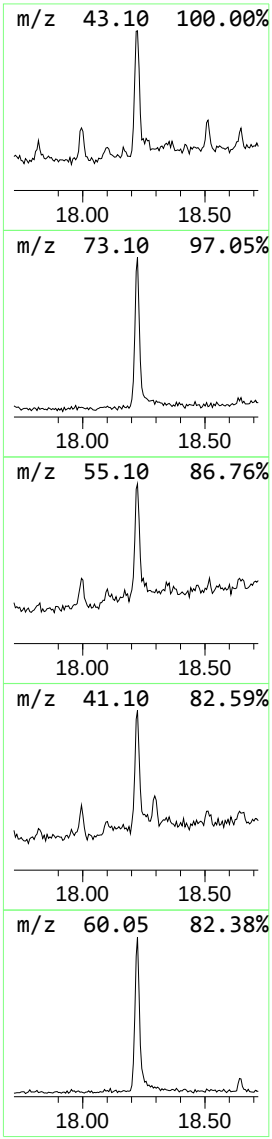
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.218	7.93 ng	293071	Phenanthrene-d10	17.330

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121721\
Data File : BM033501.D
Acq On : 17 Dec 2021 11:56
Operator : CG/JU
Sample : M5089-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-3

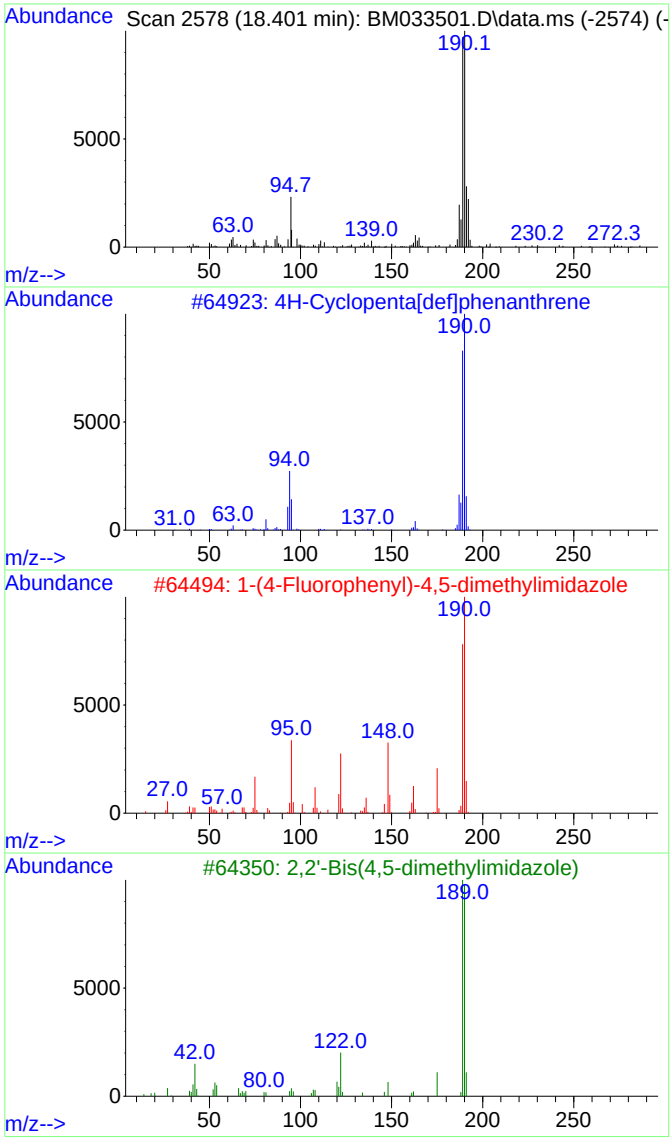
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

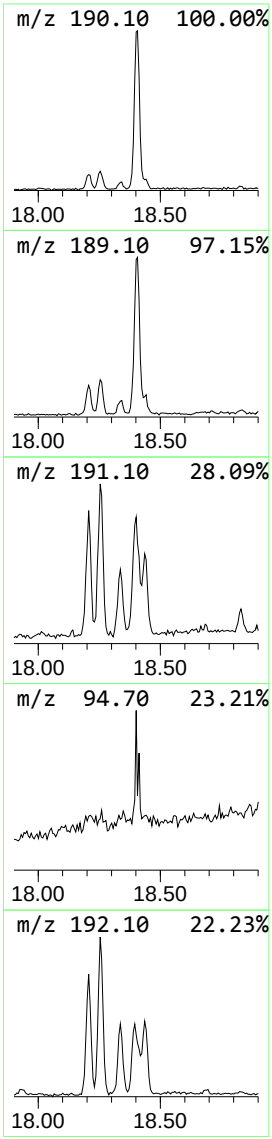
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 4H-Cyclopenta[def]phenanthrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.401	4.71 ng	174189	Phenanthrene-d10	17.330

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	81
2	1-(4-Fluorophenyl)-4,5-dimethyli...	190	C11H11FN2	1000443-18-7	53
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	52
4	1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	35
5	Cyclohexanone, 2-(2-furanylmethy...	190	C12H14O2	056053-07-7	22





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Data File : BM033501.D
Acq On : 17 Dec 2021 11:56
Operator : CG/JU
Sample : M5089-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-3

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

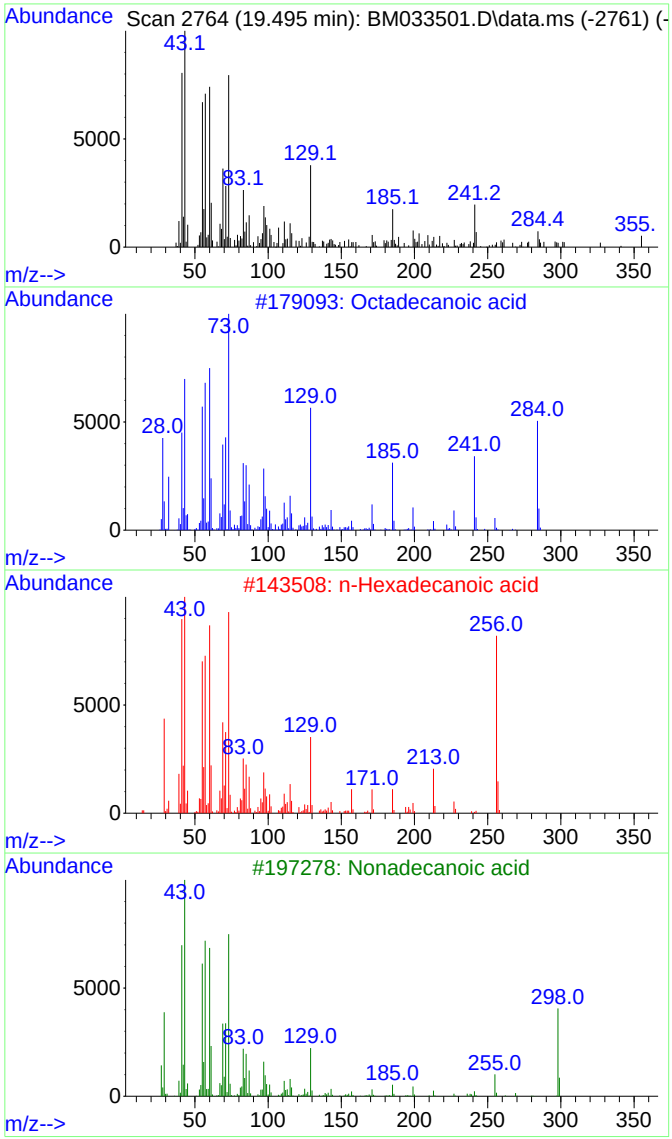
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

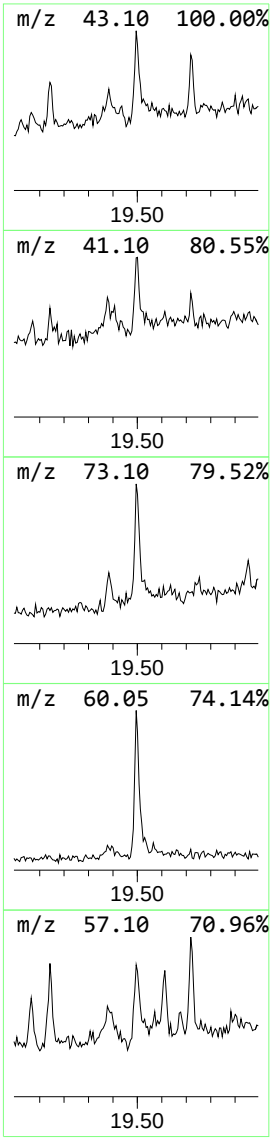
****

Peak Number 9 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.495	2.51 ng	107196	Chrysene-d12	21.506

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	80
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
3	Nonadecanoic acid	298	C19H38O2	000646-30-0	68
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58





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Data File : BM033501.D
Acq On : 17 Dec 2021 11:56
Operator : CG/JU
Sample : M5089-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-3

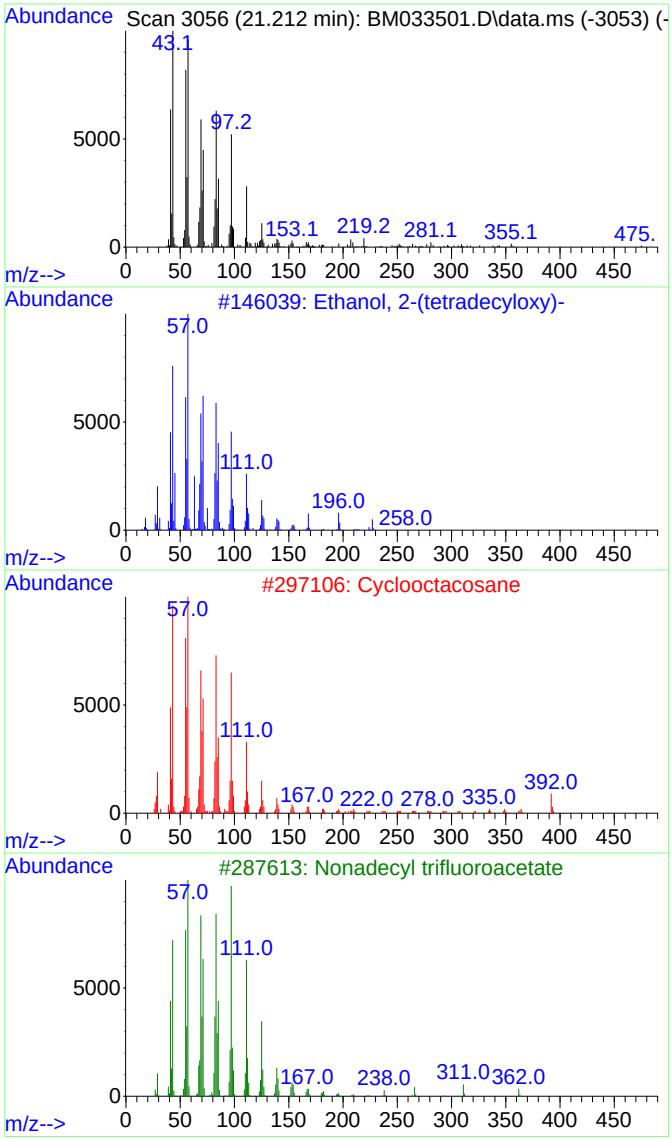
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

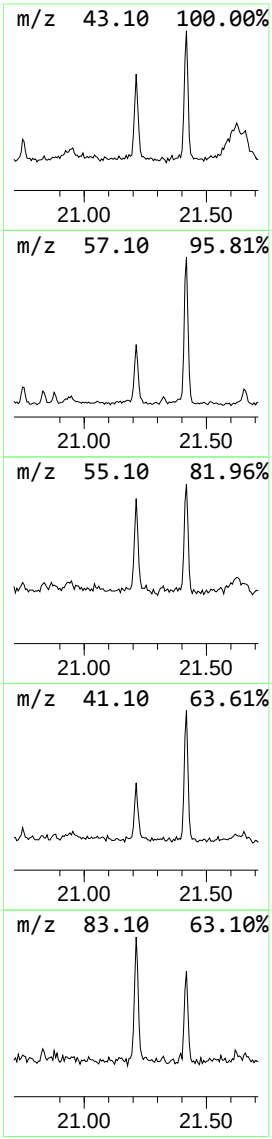
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Ethanol, 2-(tetradecyloxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.212	7.41 ng	316877	Chrysene-d12	21.506

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	93
2	Cyclooctacosane	392	C28H56	000297-24-5	91
3	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91
4	Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	91
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121721\
Data File : BM033501.D
Acq On : 17 Dec 2021 11:56
Operator : CG/JU
Sample : M5089-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-3

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
3-Penten-2-one,...	4.431	3.1	ng	52576	1	7.937	338844	20.0
2-Pentanone, 4-...	5.037	37.0	ng	626623	1	7.937	338844	20.0
2-Pentanone, 4-...	6.119	3.0	ng	50207	1	7.937	338844	20.0
Carbonic acid, ...	7.543	2.4	ng	39857	1	7.937	338844	20.0
Ethanol, 2-(2-b...	10.531	4.1	ng	102777	2	10.748	504250	20.0
Dibenzothiophene	17.148	2.5	ng	90611	4	17.330	739571	20.0
n-Hexadecanoic ...	18.218	7.9	ng	293071	4	17.330	739571	20.0
4H-Cyclopenta[d...	18.401	4.7	ng	174189	4	17.330	739571	20.0
Octadecanoic acid	19.495	2.5	ng	107196	5	21.506	854876	20.0
Ethanol, 2-(tet...	21.212	7.4	ng	316877	5	21.506	854876	20.0