LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM051922\
Data File : BM035156.D
Acq On : 19 May 2022 17:01
Operator : CG/JU
Sample : N2865-12
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P019-SS001-1824-01

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-BM042722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM035156.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.622	87	91	103	rVB	130230	182215	3.05%	0.469%
2	5.481	400	407	421	rBV	2409152	3424124	57.29%	8.821%
3	7.075	670	678	694	rBV	2281543	3553825	59.46%	9.155%
4	7.904	813	819	827	rBV	546105	849709	14.22%	2.189%
5	9.063	1008	1016	1031	rBV	1389091	2281456	38.17%	5.877%
6	10.704	1288	1295	1307	rBV	666478	1133202	18.96%	2.919%
7	13.169	1707	1714	1724	rBV	3218500	4514322	75.53%	11.630%
8	13.745	1807	1812	1822	rBV	104975	146968	2.46%	0.379%
9	13.874	1829	1834	1842	rBV4	36480	64221	1.07%	0.165%
10	13.998	1850	1855	1864	rVB	64094	92936	1.55%	0.239%
11	14.169	1875	1884	1897	rBV	100599	172123	2.88%	0.443%
12	14.539	1940	1947	1955	rBV	1053000	1543254	25.82%	3.976%
13	14.651	1962	1966	1973	rVB5	34091	64054	1.07%	0.165%
14	14.963	2012	2019	2027	rVV2	39634	74248	1.24%	0.191%
15	16.027	2194	2200	2208	rBV	2616721	3585691	59.99%	9.237%
16	16.539	2282	2287	2293	rBV2	43851	65755	1.10%	0.169%
17	17.286	2408	2414	2419	rBV	1100427	1563254	26.16%	4.027%
18	17.327	2419	2421	2428	rVB	53840	68713	1.15%	0.177%
19	17.680	2475	2481	2492	rVB3	87521	140097	2.34%	0.361%
20	17.968	2525	2530	2535	rBV	161125	196779	3.29%	0.507%
21	18.192	2562	2568	2576	rBV	632081	903283	15.11%	2.327%
22	18.257	2576	2579	2584	rVB	68881	97052	1.62%	0.250%
23	19.051	2709	2714	2722	rBV	302061	422788	7.07%	1.089%
24	19.139	2725	2729	2733	rVB	122023	139642	2.34%	0.360%
25	19.274	2748	2752	2756	rBV	198957	217118	3.63%	0.559%
26	19.345	2756	2764	2766	rVV2	210424	370882	6.21%	0.955%
27	19.368	2766	2768	2779	rVV	268838	360980	6.04%	0.930%
28	19.468	2780	2785	2797	rVV	416021	618775	10.35%	1.594%
29	19.598	2803	2807	2816	rBV8	69863	153802	2.57%	0.396%
30	19.704	2822	2825	2830	rBV	80756	103784	1.74%	0.267%
31	19.827	2842	2846	2852	rBV3	83529	123537	2.07%	0.318%
32	19.909	2855	2860	2869	rVB	4797830	5976681	100.00%	15.397%
33	20.198	2906	2909	2913	rVB5	53493	60093	1.01%	0.155%
34	20.409	2942	2945	2950	rBV	91131	126017	2.11%	0.325%
35	21.186	3073	3077	3085	rBV	532521	626059	10.48%	1.613%
36	21.392	3108	3112	3119	rBV	909108	970736	16.24%	2.501%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM051922\
Data File : BM035156.D
Acq On : 19 May 2022 17:01
Operator : CG/JU
Sample : N2865-12
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P019-SS001-1824-01

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-BM042722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.468	3120	3125	3130	rBV	1446044	1874275	31.36%	4.828%
38	23.856	3525	3531	3543	rVB2	937779	1955240	32.71%	5.037%

Sum of corrected areas: 38817690

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM051922\
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Acq On : 19 May 2022 17:01
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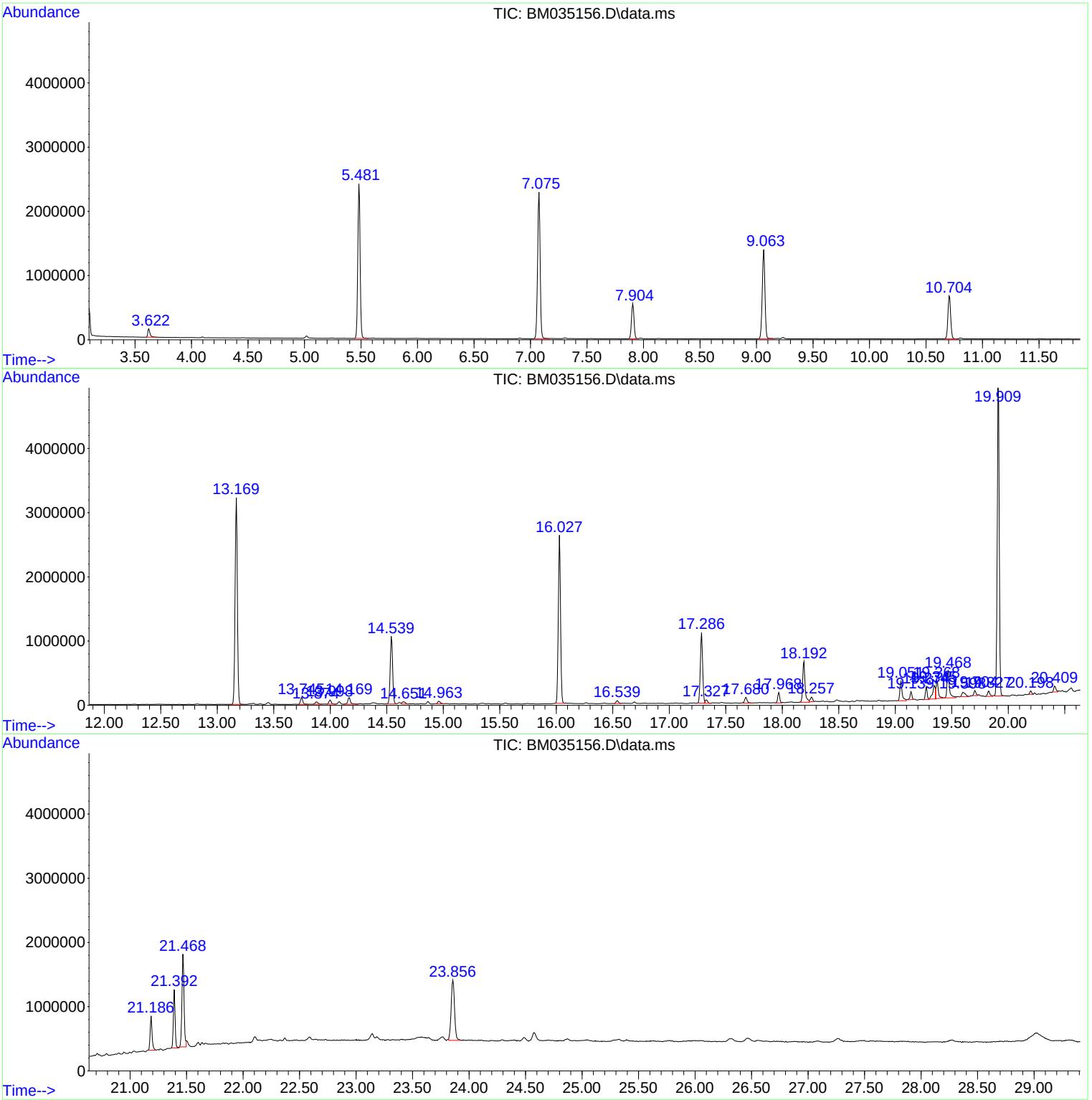
Sample : N2865-12
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P019-SS001-1824-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.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\BM051922\
Data File : BM035156.D
Acq On : 19 May 2022 17:01
Operator : CG/JU
Sample : N2865-12
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P019-SS001-1824-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

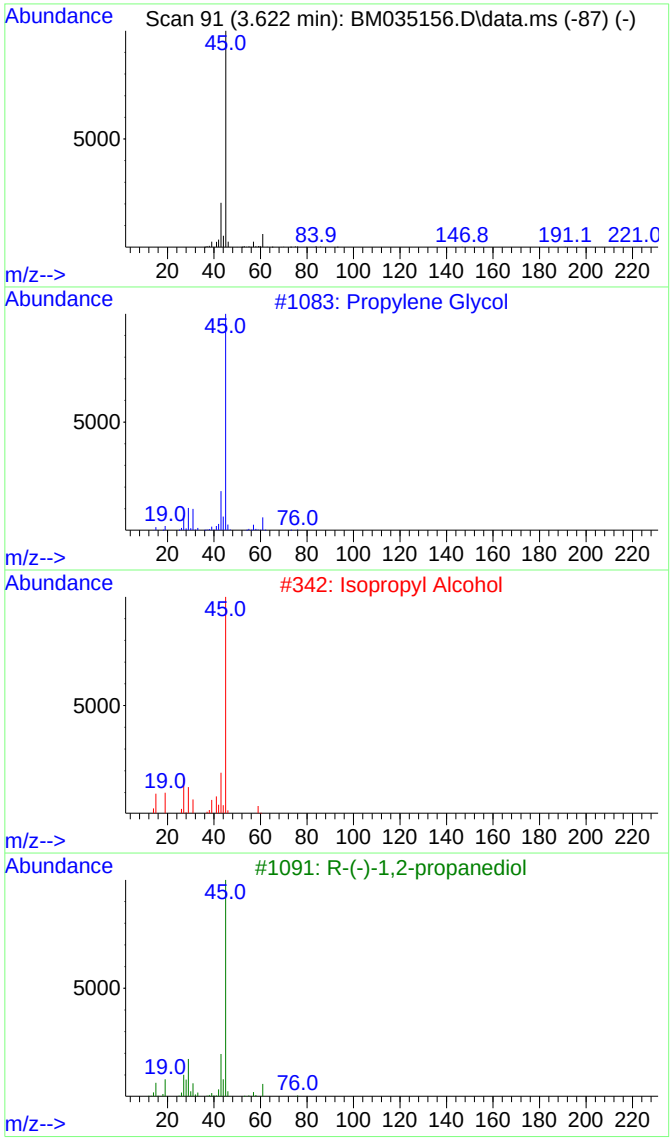
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

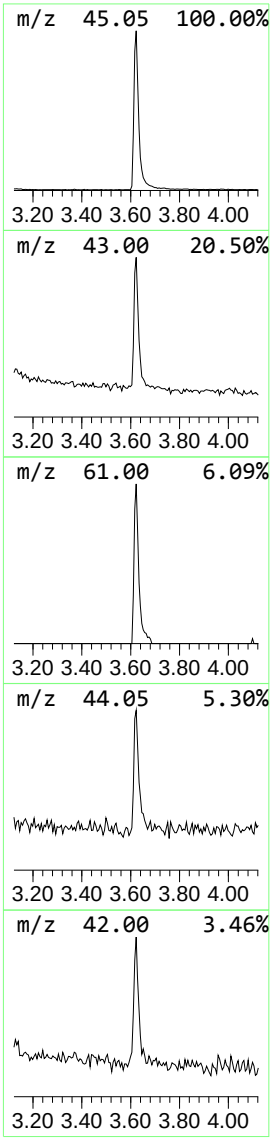
****

Peak Number 1 Propylene Glycol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.622	4.29 ng	182215	1,4-Dichlorobenzene-d4	7.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	78
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	56
3	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
4	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9
5	2-Heptanol, (S)-	116	C7H16O	006033-23-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM051922\
Data File : BM035156.D
Acq On : 19 May 2022 17:01
Operator : CG/JU
Sample : N2865-12
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P019-SS001-1824-01

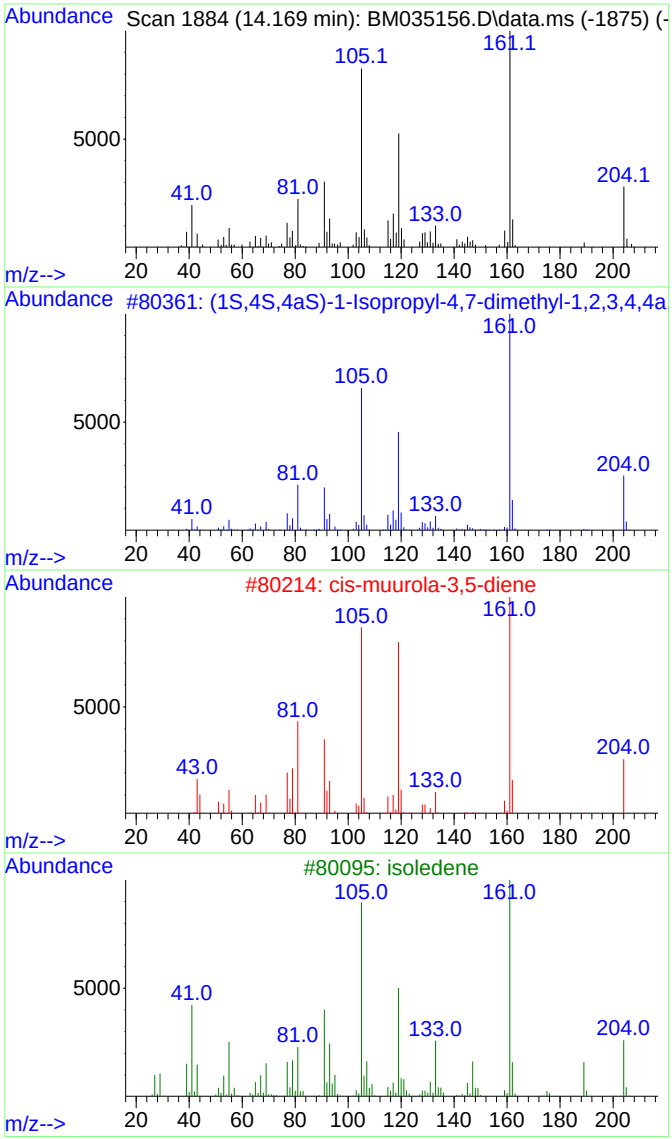
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

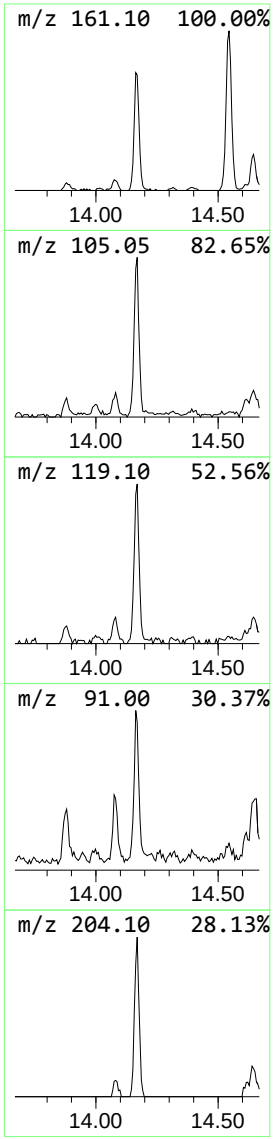
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 (1S,4S,4aS)-1-Isopropyl-4,7... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.169	2.23 ng	172123	Acenaphthene-d10	14.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1S,4S,4aS)-1-Isopropyl-4,7-dime...	204	C15H24	267665-20-3	98
2	cis-muurola-3,5-diene	204	C15H24	1000365-95-4	91
3	isoledene	204	C15H24	095910-36-4	83
4	.alpha.-Cubebene	204	C15H24	017699-14-8	80
5	Naphthalene, 1,2,3,5,6,8a-hexahy...	204	C15H24	000483-76-1	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM051922\
Data File : BM035156.D
Acq On : 19 May 2022 17:01
Operator : CG/JU
Sample : N2865-12
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P019-SS001-1824-01

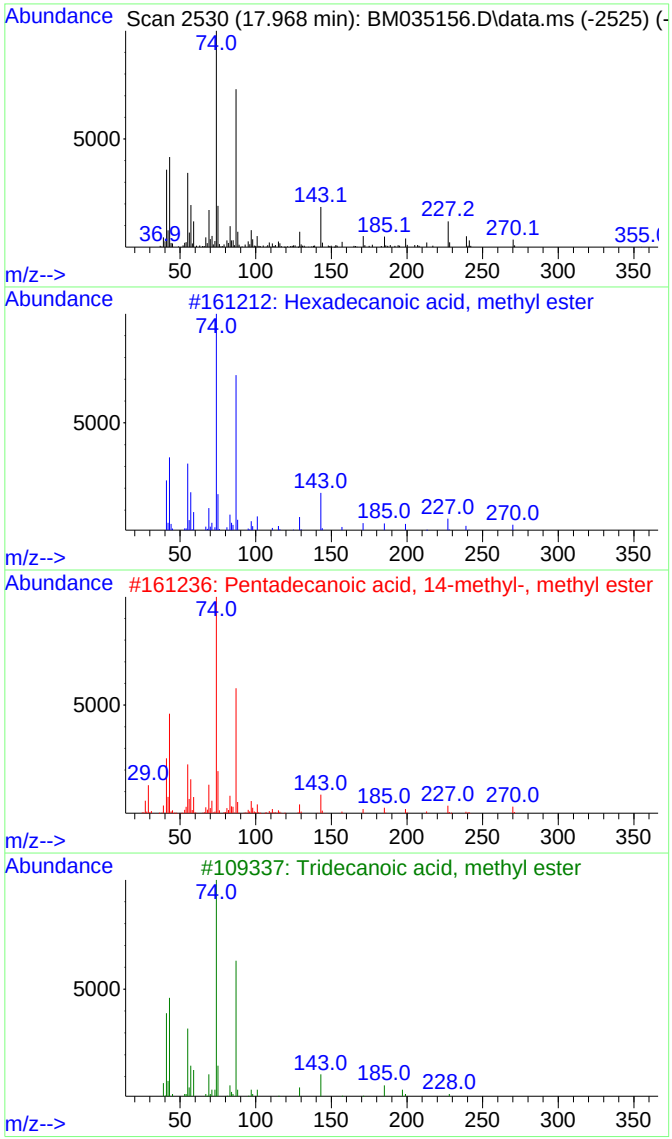
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

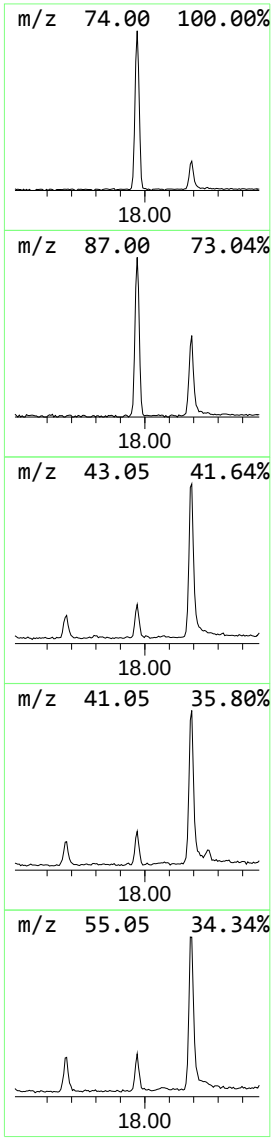
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Hexadecanoic acid, methyl e... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.968	2.52 ng	196779	Phenanthrene-d10	17.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	96
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	93
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
4	Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM051922\
Data File : BM035156.D
Acq On : 19 May 2022 17:01
Operator : CG/JU
Sample : N2865-12
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P019-SS001-1824-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

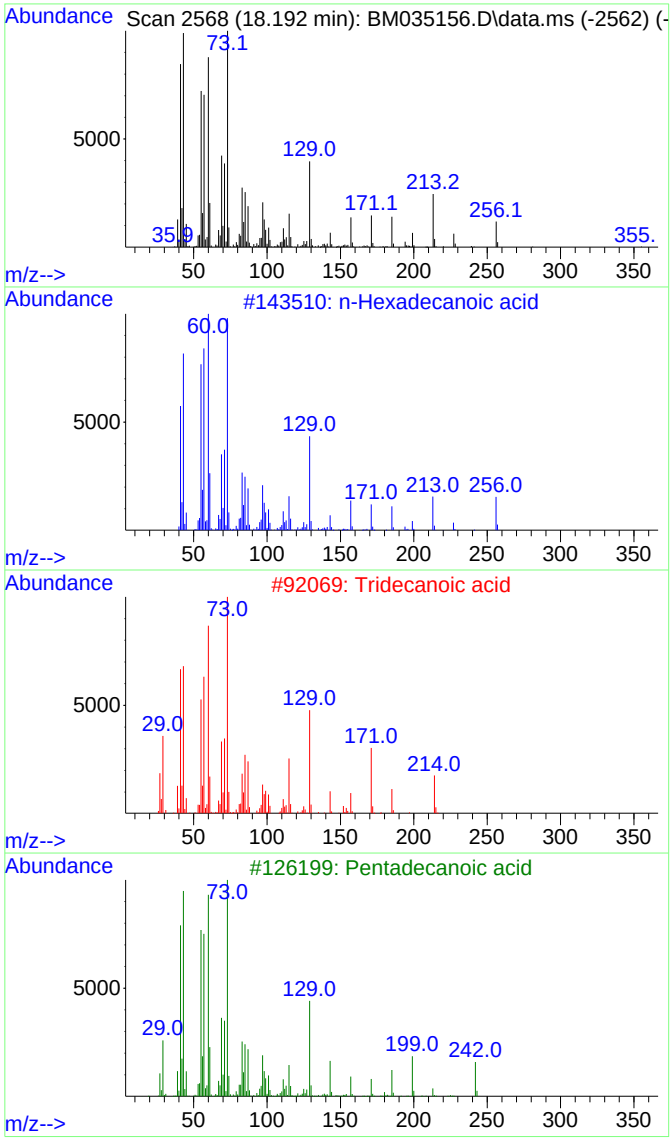
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

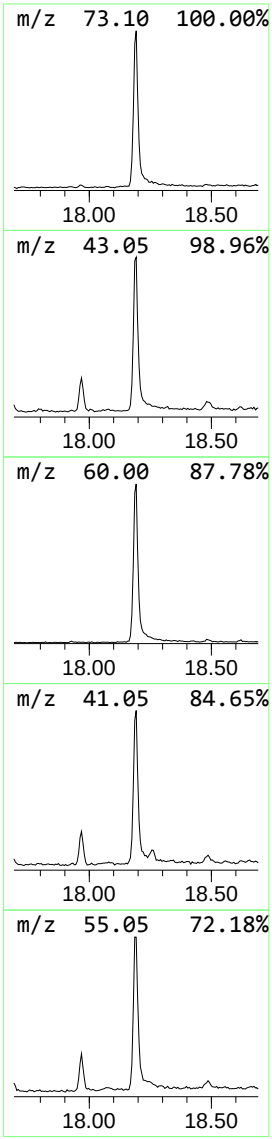
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.192	11.56 ng	903283	Phenanthrene-d10	17.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
5	Octadecanoic acid	284	C18H36O2	000057-11-4	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM051922\
Data File : BM035156.D
Acq On : 19 May 2022 17:01
Operator : CG/JU
Sample : N2865-12
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P019-SS001-1824-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

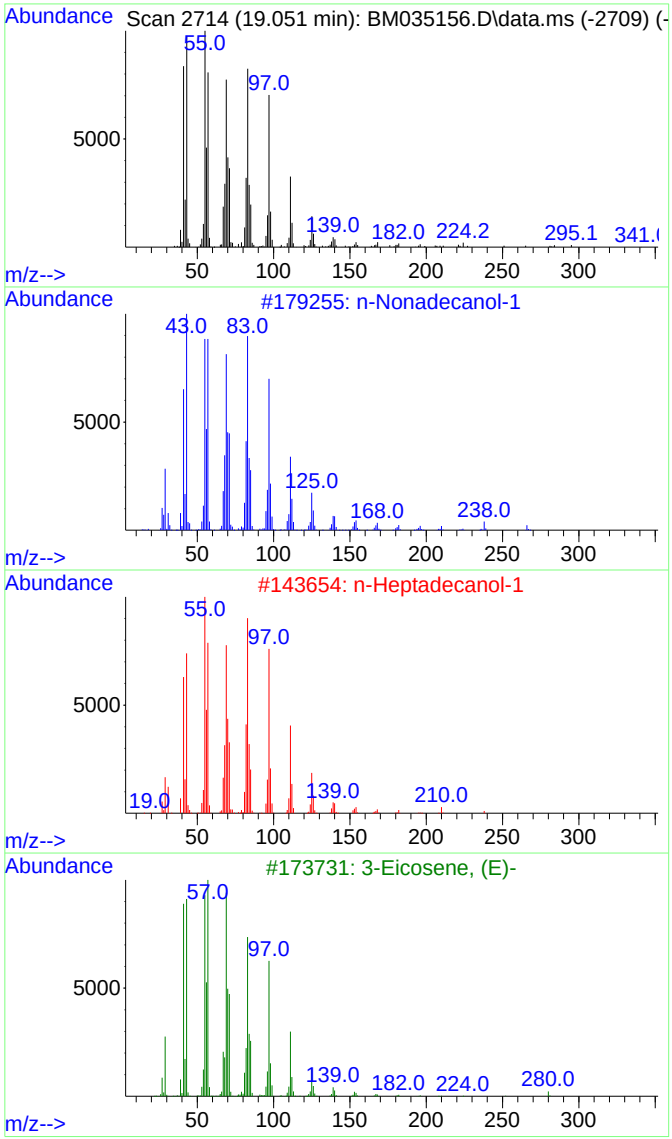
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

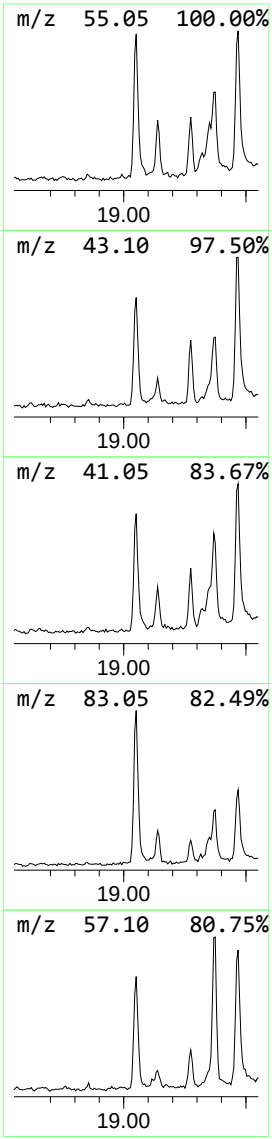
****

Peak Number 5 n-Nonadecanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.051	5.41 ng	422788	Phenanthrene-d10	17.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
2	n-Heptadecanol-1	256	C17H36O	001454-85-9	95
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	94
4	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	94
5	Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	94





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Data File : BM035156.D
Acq On : 19 May 2022 17:01
Operator : CG/JU
Sample : N2865-12
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P019-SS001-1824-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

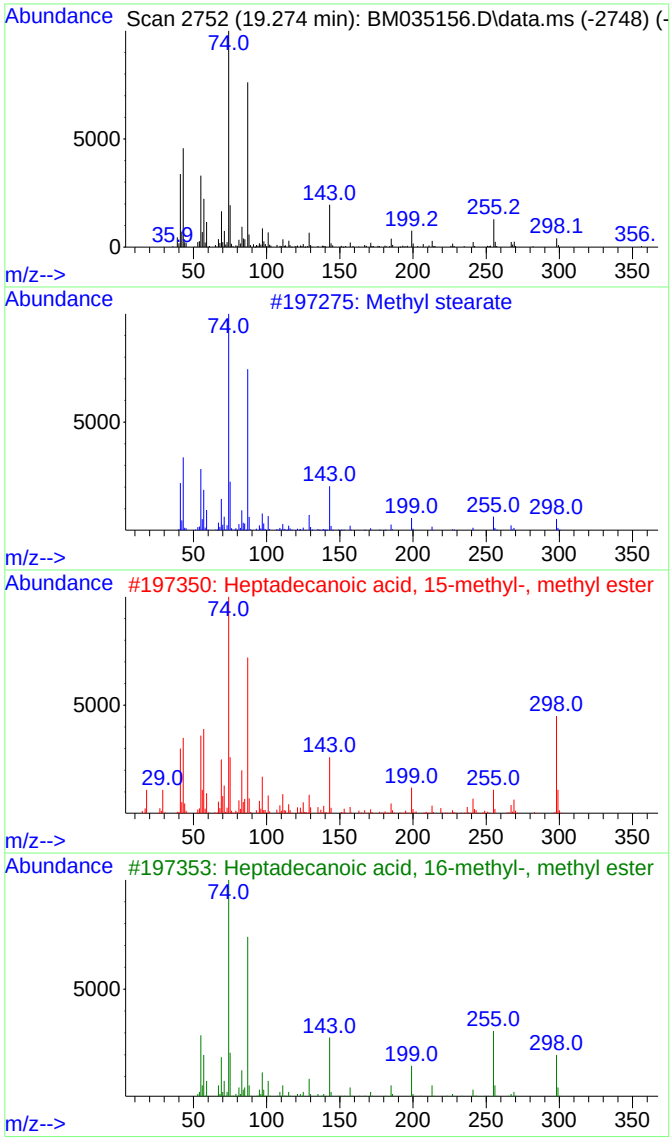
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

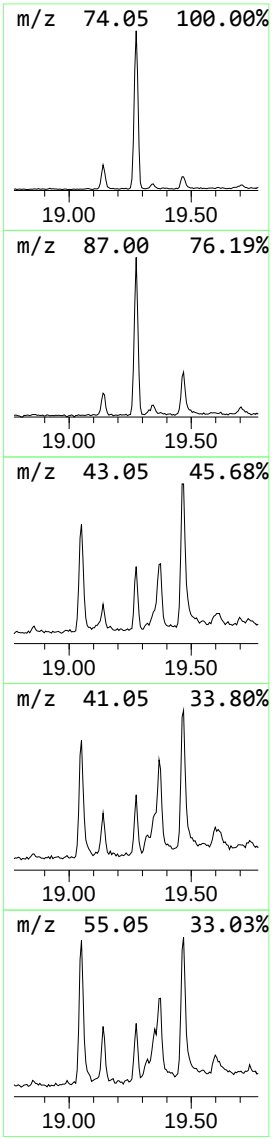
****

Peak Number 6 Methyl stearate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.274	2.78 ng	217118	Phenanthrene-d10	17.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	98
2	Heptadecanoic acid, 15-methyl-, ...	298	C19H38O2	054833-55-5	94
3	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	94
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
5	Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM051922\
Data File : BM035156.D
Acq On : 19 May 2022 17:01
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Sample : N2865-12
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P019-SS001-1824-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

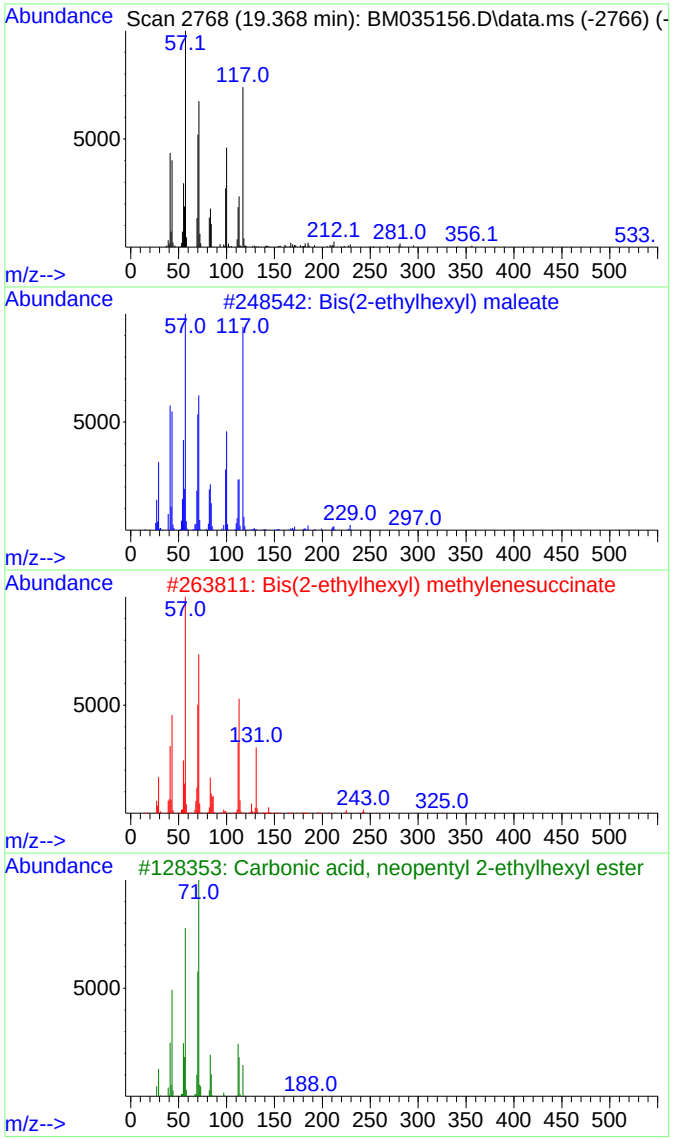
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

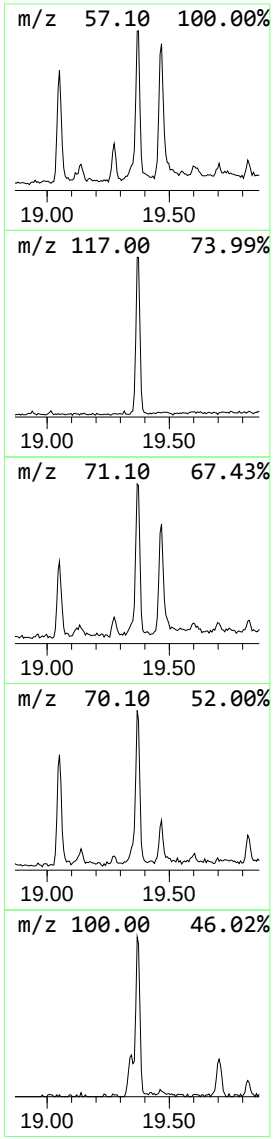
****

Peak Number 8 Bis(2-ethylhexyl) maleate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.368	4.62 ng	360980	Phenanthrene-d10	17.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bis(2-ethylhexyl) maleate	340	C20H36O4	000142-16-5	90
2	Bis(2-ethylhexyl) methylenesucci...	354	C21H38O4	002287-83-4	38
3	Carbonic acid, neopentyl 2-ethyl...	244	C14H28O3	1000357-85-7	35
4	Oxalic acid, 2-ethylhexyl ethyl ...	230	C12H22O4	1000309-38-4	27
5	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	27





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Data File : BM035156.D
Acq On : 19 May 2022 17:01
Operator : CG/JU
Sample : N2865-12
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P019-SS001-1824-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

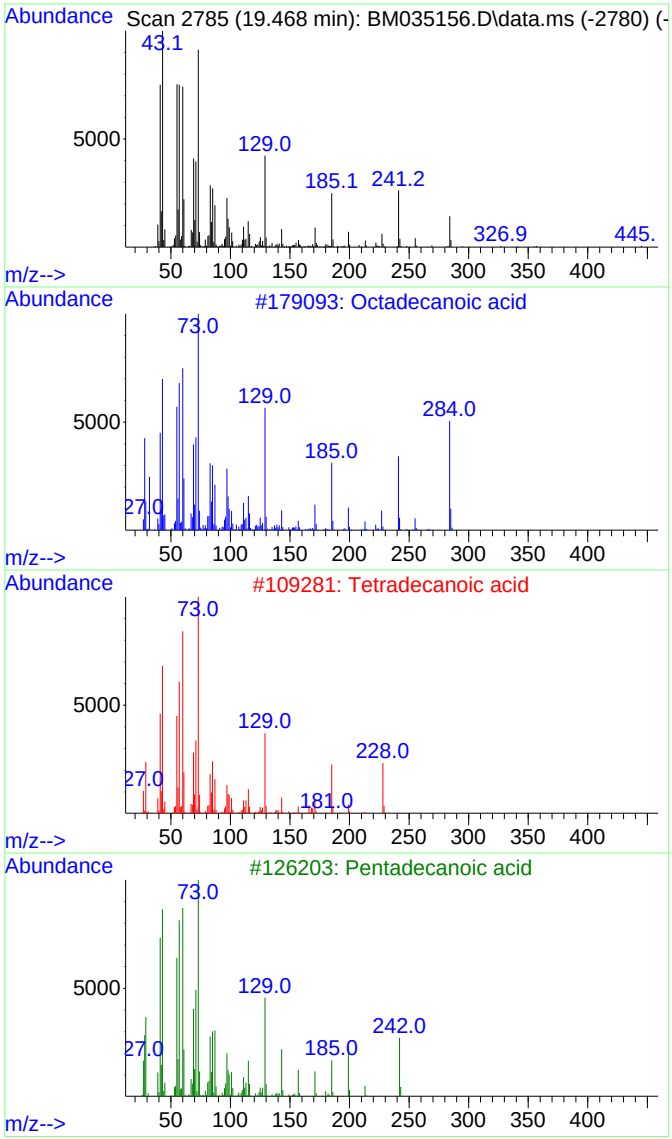
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

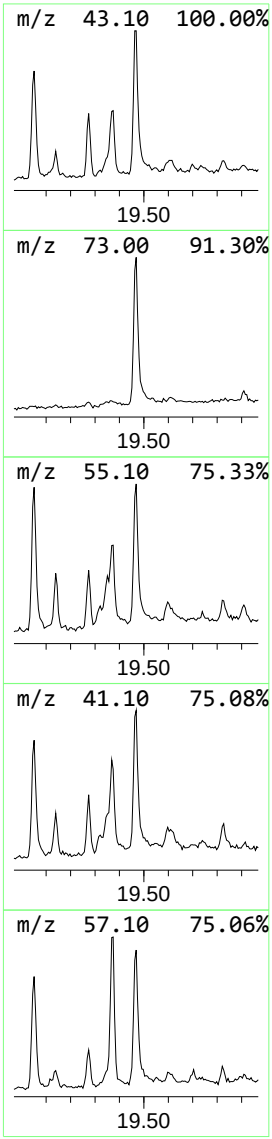
****

Peak Number 9 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.468	6.60 ng	618775	Chrysene-d12	21.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM051922\
Data File : BM035156.D
Acq On : 19 May 2022 17:01
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ALS Vial : 7 Sample Multiplier: 1

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BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.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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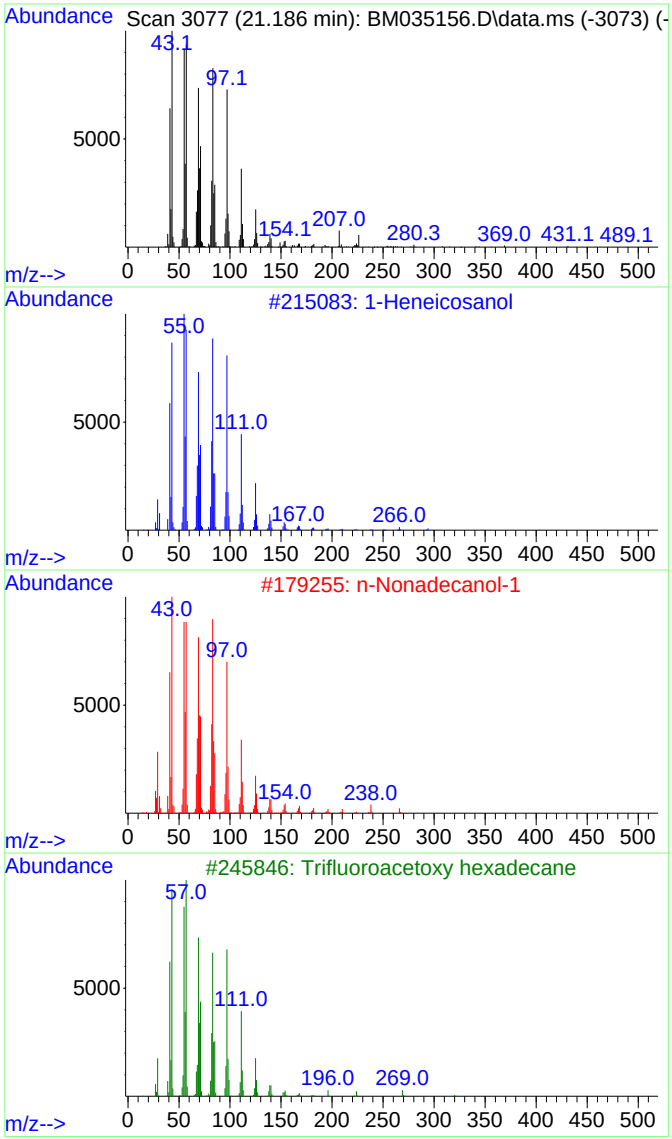
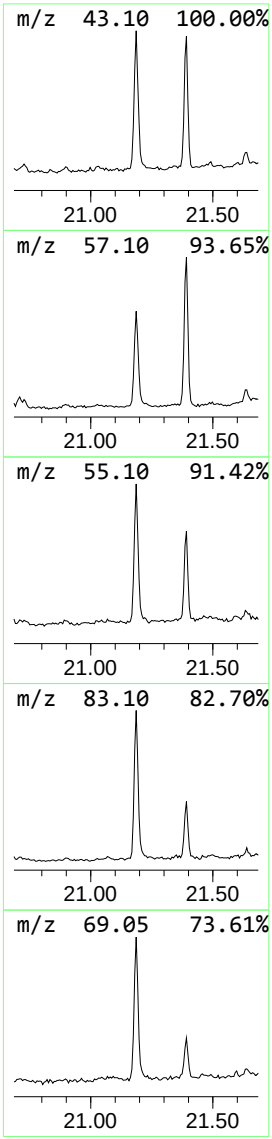
Peak Number 10 1-Heneicosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.186	6.68 ng	626059	Chrysene-d12	21.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5	Pentacos-1-ene	350	C25H50	016980-85-1	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM051922\
Data File : BM035156.D
Acq On : 19 May 2022 17:01
Operator : CG/JU
Sample : N2865-12
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P019-SS001-1824-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.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
Propylene Glycol	3.622	4.3	ng	182215	1	7.904	849709	20.0
(1S,4S,4aS)-1-I...	14.169	2.2	ng	172123	3	14.539	1543250	20.0
Hexadecanoic ac...	17.968	2.5	ng	196779	4	17.286	1563250	20.0
n-Hexadecanoic ...	18.192	11.6	ng	903283	4	17.286	1563250	20.0
n-Nonadecanol-1	19.051	5.4	ng	422788	4	17.286	1563250	20.0
Methyl stearate	19.274	2.8	ng	217118	4	17.286	1563250	20.0
Bis(2-ethylhexy...	19.368	4.6	ng	360980	4	17.286	1563250	20.0
Octadecanoic acid	19.468	6.6	ng	618775	5	21.468	1874280	20.0
1-Heneicosanol	21.186	6.7	ng	626059	5	21.468	1874280	20.0