LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030222\
Data File : BF127147.D
Acq On : 02 Mar 2022 15:12
Operator : CG\JU
Sample : N1725-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-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_F\Methods\8270-BF021622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127147.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.110	477	480	490	rVB	132874	147956	4.37%	0.837%
2	5.516	545	549	552	rBV	1293168	1184294	34.95%	6.704%
3	6.187	660	663	676	rVB	125332	98530	2.91%	0.558%
4	6.516	715	719	725	rVB	969936	897575	26.49%	5.081%
5	6.887	779	782	786	rBV	703844	573737	16.93%	3.248%
6	6.945	788	792	796	rBV	35208	40936	1.21%	0.232%
7	7.457	873	879	882	rBV	1916763	1906327	56.25%	10.791%
8	7.534	887	892	902	rVB3	35950	58255	1.72%	0.330%
9	7.892	948	953	959	rBV	43008	58695	1.73%	0.332%
10	8.069	979	983	992	rBV	109571	133428	3.94%	0.755%
11	8.169	996	1000	1003	rBV	810891	773444	22.82%	4.378%
12	8.528	1051	1061	1065	rBV	281632	402435	11.87%	2.278%
13	8.586	1068	1071	1081	rVB3	26302	44793	1.32%	0.254%
14	9.251	1178	1184	1187	rBV	4005599	3388980	100.00%	19.183%
15	9.586	1237	1241	1247	rBV2	72578	91662	2.70%	0.519%
16	9.739	1264	1267	1274	rBV4	43375	76089	2.25%	0.431%
17	9.792	1274	1276	1281	rVB	42915	41048	1.21%	0.232%
18	9.933	1296	1300	1303	rVB	949884	853280	25.18%	4.830%
19	10.304	1361	1363	1365	rBV	65762	57422	1.69%	0.325%
20	10.345	1368	1370	1374	rVB2	80635	67415	1.99%	0.382%
21	10.722	1430	1434	1437	rBV	1924165	1666921	49.19%	9.436%
22	11.363	1540	1543	1546	rVB	146338	115756	3.42%	0.655%
23	11.422	1549	1553	1556	rBV	1052707	845472	24.95%	4.786%
24	11.580	1576	1580	1588	rBV	89341	117029	3.45%	0.662%
25	11.974	1644	1647	1650	rBV	81087	59337	1.75%	0.336%
26	12.786	1781	1785	1788	rVB3	29140	40233	1.19%	0.228%
27	12.892	1801	1803	1811	rVB2	62528	61155	1.80%	0.346%
28	13.010	1818	1823	1826	rBV	3294623	2714867	80.11%	15.367%
29	13.927	1971	1979	1989	rBV5	58768	156310	4.61%	0.885%
30	14.068	1999	2003	2006	rVB	461213	426236	12.58%	2.413%
31	15.562	2251	2257	2266	rBV	367802	469307	13.85%	2.656%
32	16.533	2418	2422	2434	rVB	18856	52499	1.55%	0.297%
33	17.727	2618	2625	2629	rBV10	15956	45014	1.33%	0.255%

Sum of corrected areas: 17666437

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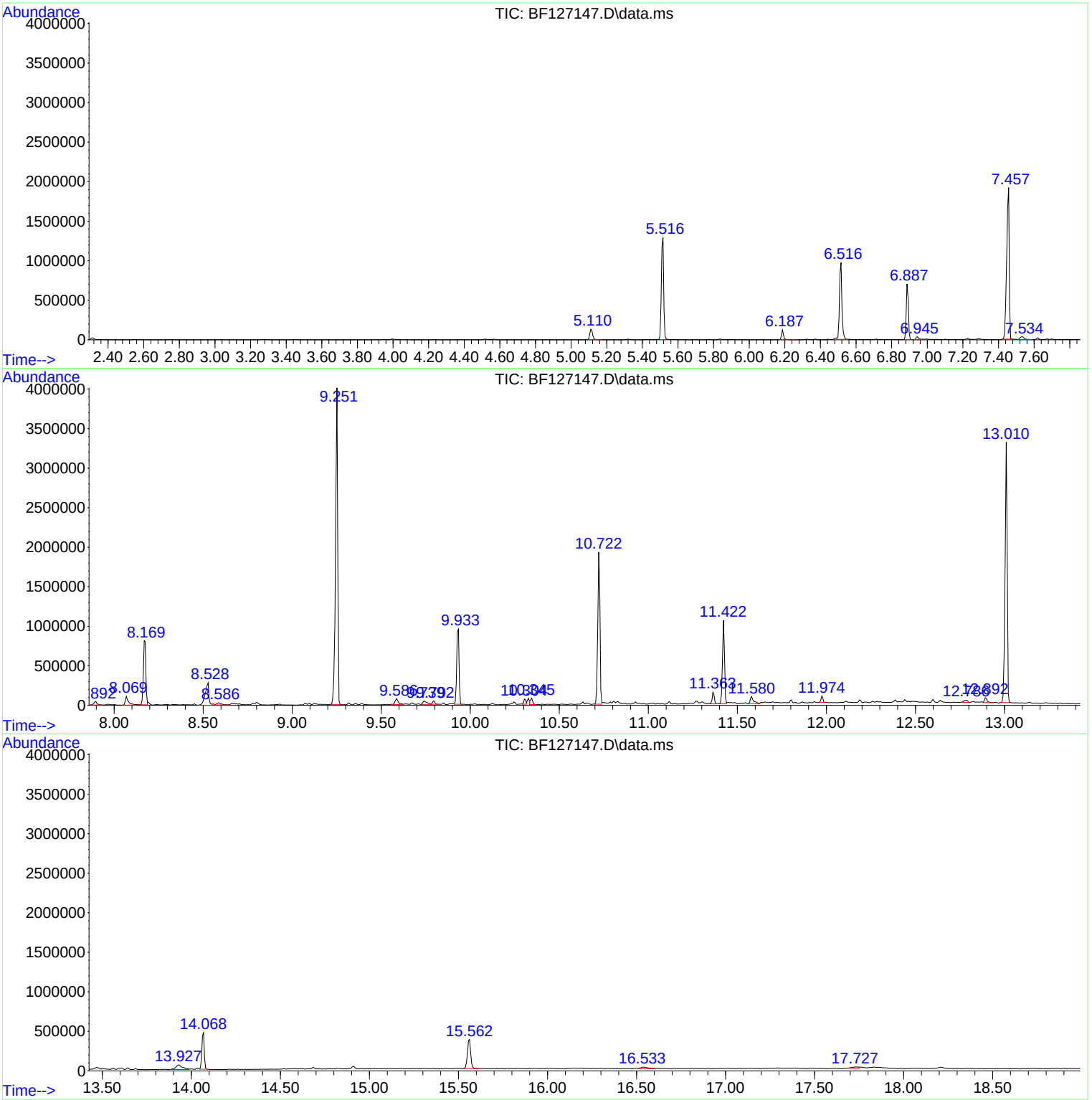
BNA_F
ClientSampleId :
MW-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.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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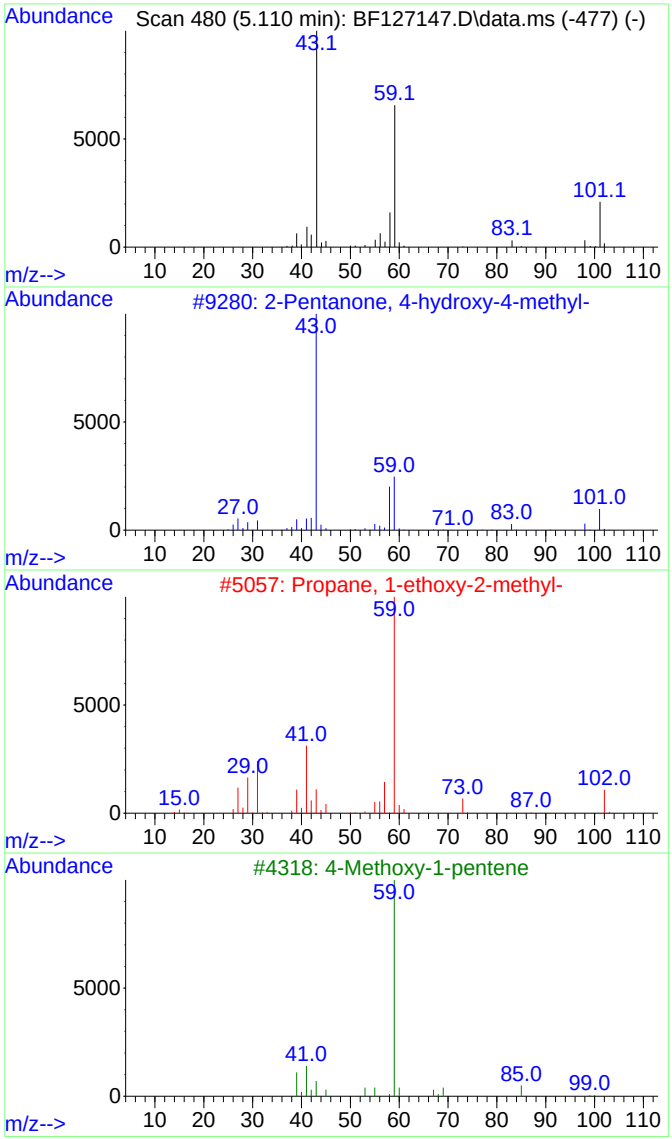
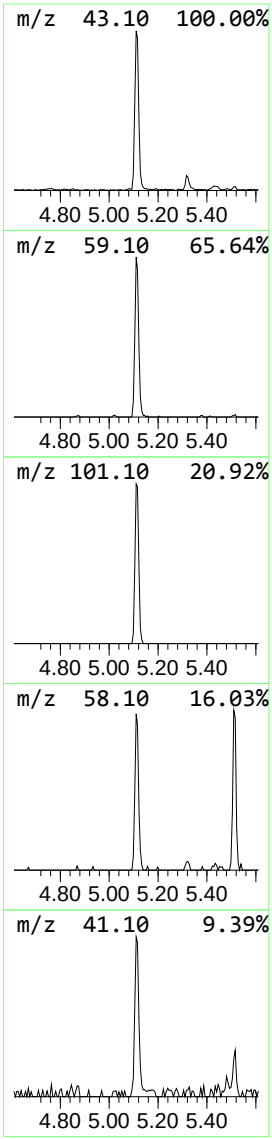
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	5.16 ng	147956	1,4-Dichlorobenzene-d4	6.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	38
3	4-Methoxy-1-pentene	100	C6H12O	098386-09-5	35
4	2,3-Dimethyloxirane-2-carboxylic...	130	C6H10O3	1000306-64-4	23
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17





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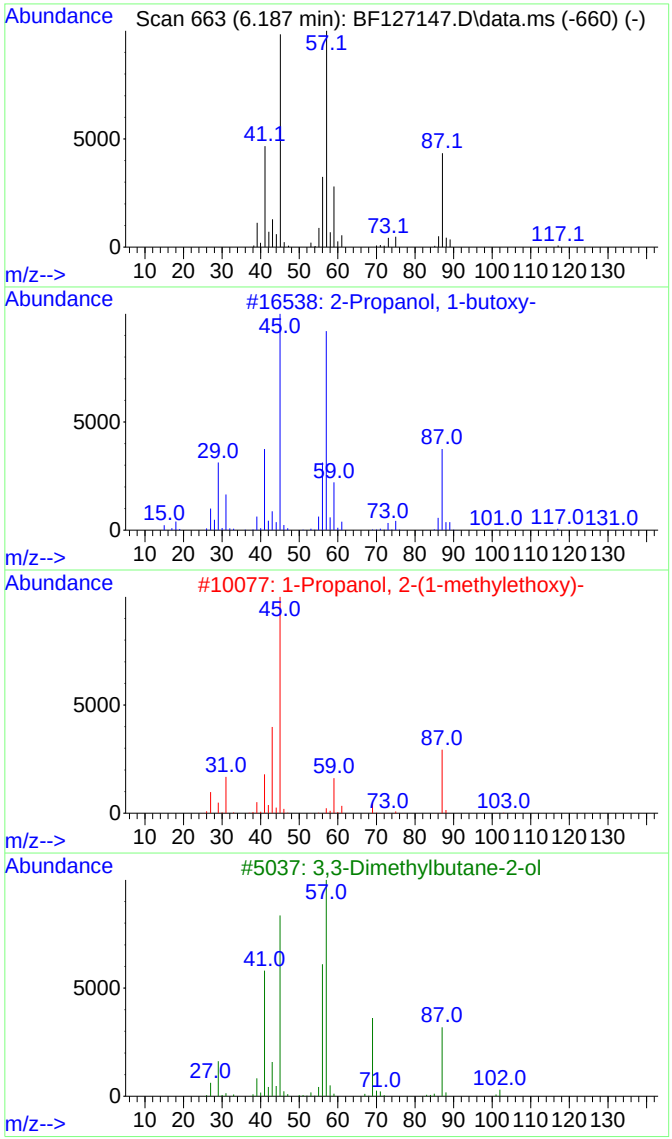
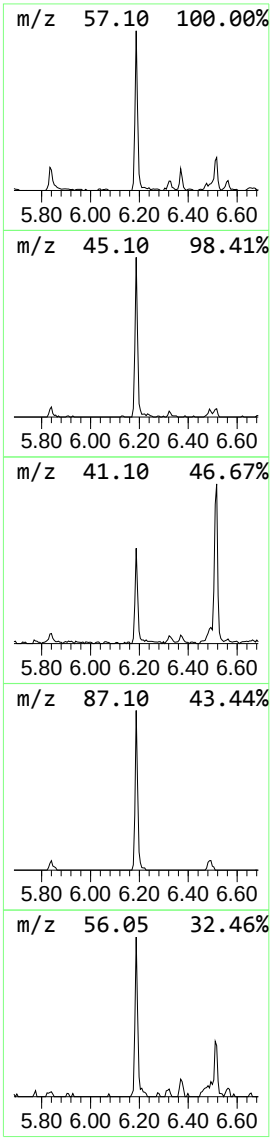
****

Peak Number 2 2-Propanol, 1-butoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.187	3.43 ng	98530	1,4-Dichlorobenzene-d4	6.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	90
2	1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	59
3	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	42
4	Hexane, 1,2,3-trimethoxy-	176	C9H20O3	020637-29-0	40
5	Formic acid, 1-methylpropyl ester	102	C5H10O2	000589-40-2	40





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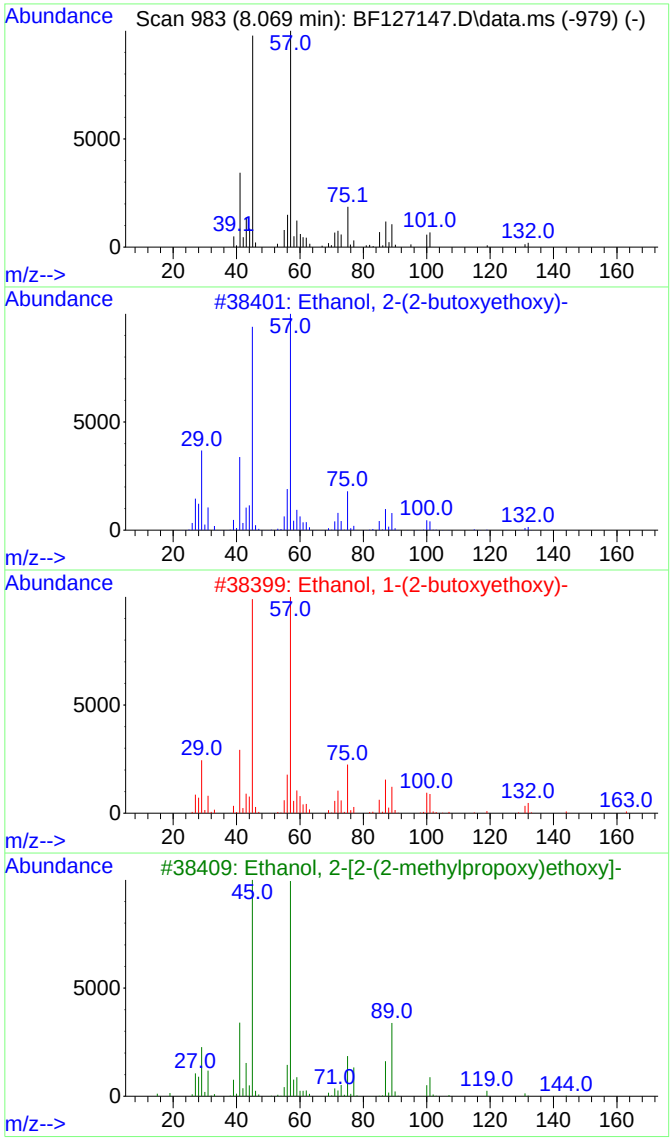
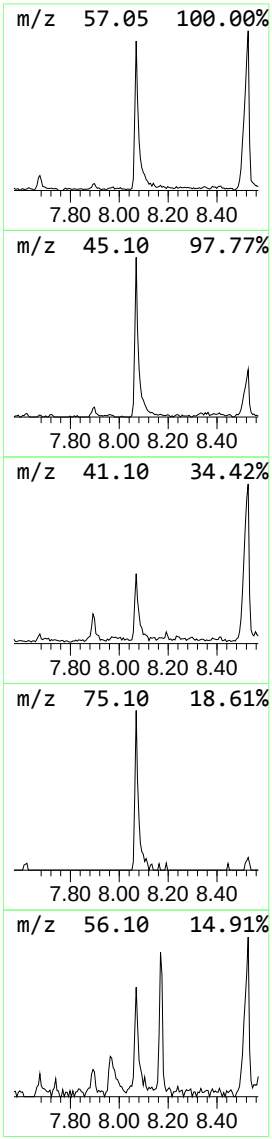
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.069	3.45 ng	133428	Naphthalene-d8	8.175

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	83
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
5	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53





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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
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TIC Library : C:\Database\NIST20.L
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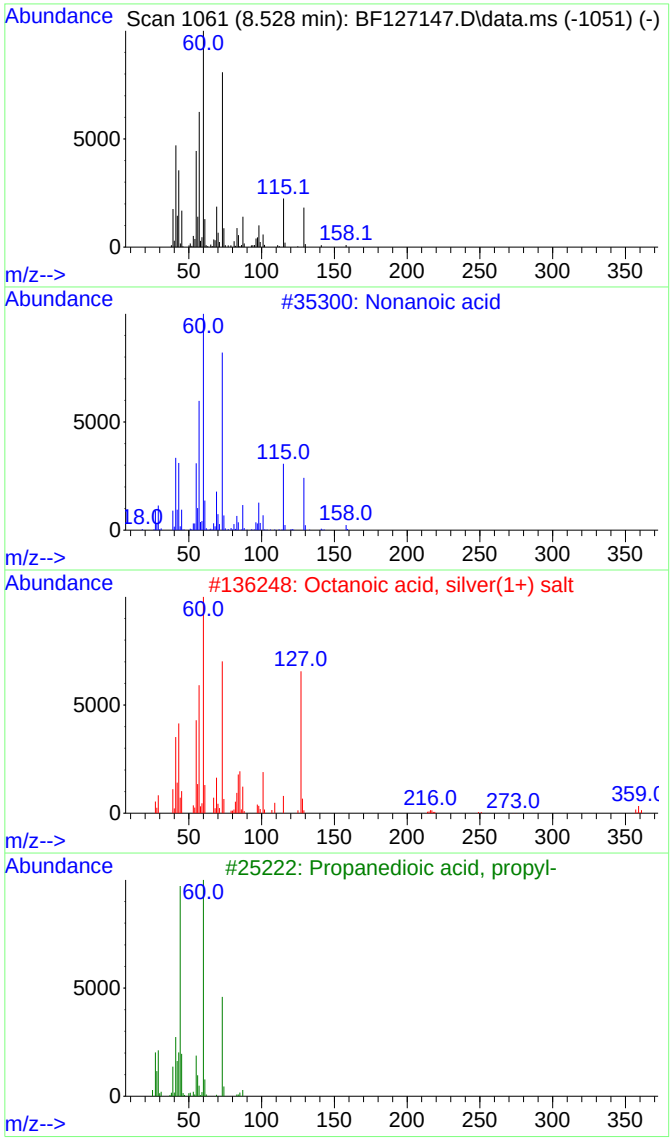
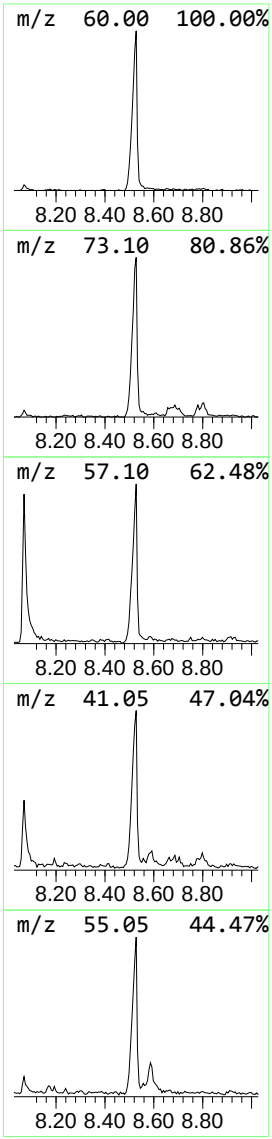
****

Peak Number 4 Nonanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.528	10.41 ng	402435	Naphthalene-d8	8.175

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanoic acid	158	C9H18O2	000112-05-0	96
2	Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	53
3	Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	50
4	Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	47
5	Pentanoic acid	102	C5H10O2	000109-52-4	47





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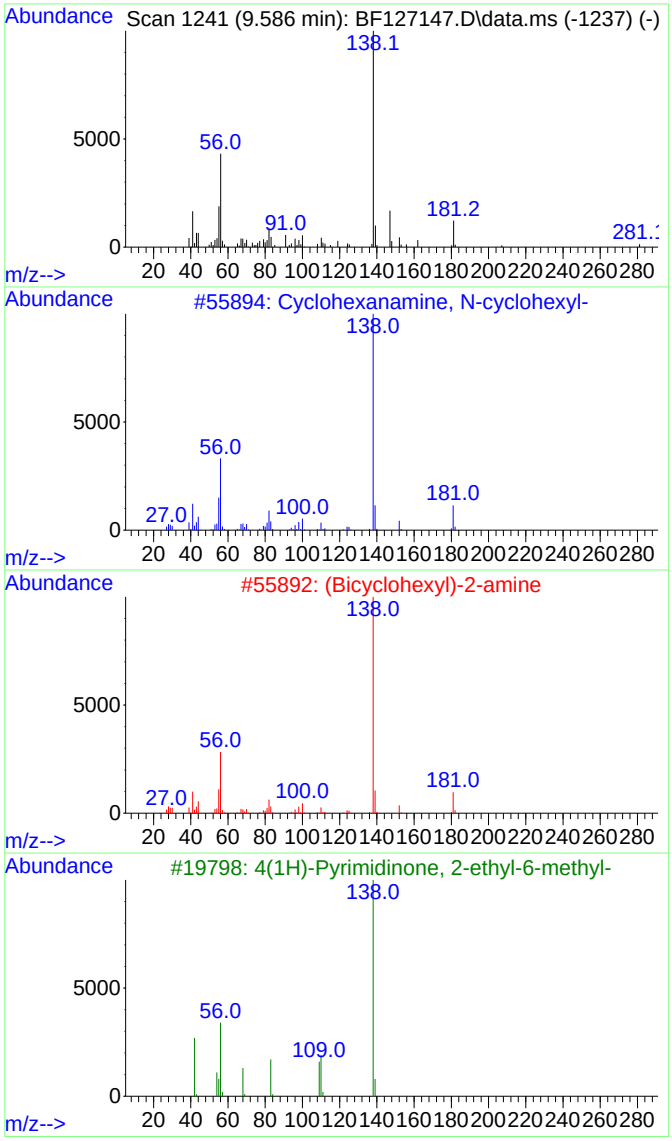
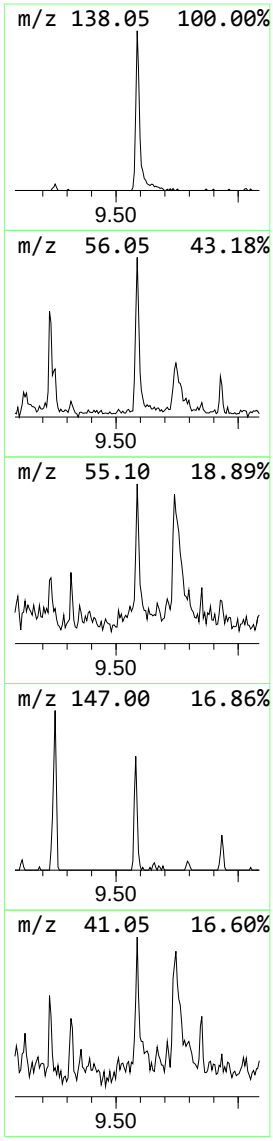
****
Peak Number 5 Cyclohexanamine, N-cyclohexyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.586	2.15 ng	91662	Acenaphthene-d10	9.933

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanamine, N-cyclohexyl-	181	C12H23N	000101-83-7	93
2	(Bicyclohexyl)-2-amine	181	C12H23N	006283-14-3	81
3	4(1H)-Pyrimidinone, 2-ethyl-6-me...	138	C7H10N2O	016858-50-7	59
4	1H-Pyrazole-3-carboxylic acid (m...	278	C15H26N4O	1000303-25-6	50
5	Butanoic acid, 4-dicyclohexylami...	281	C16H27NO3	328013-95-2	50





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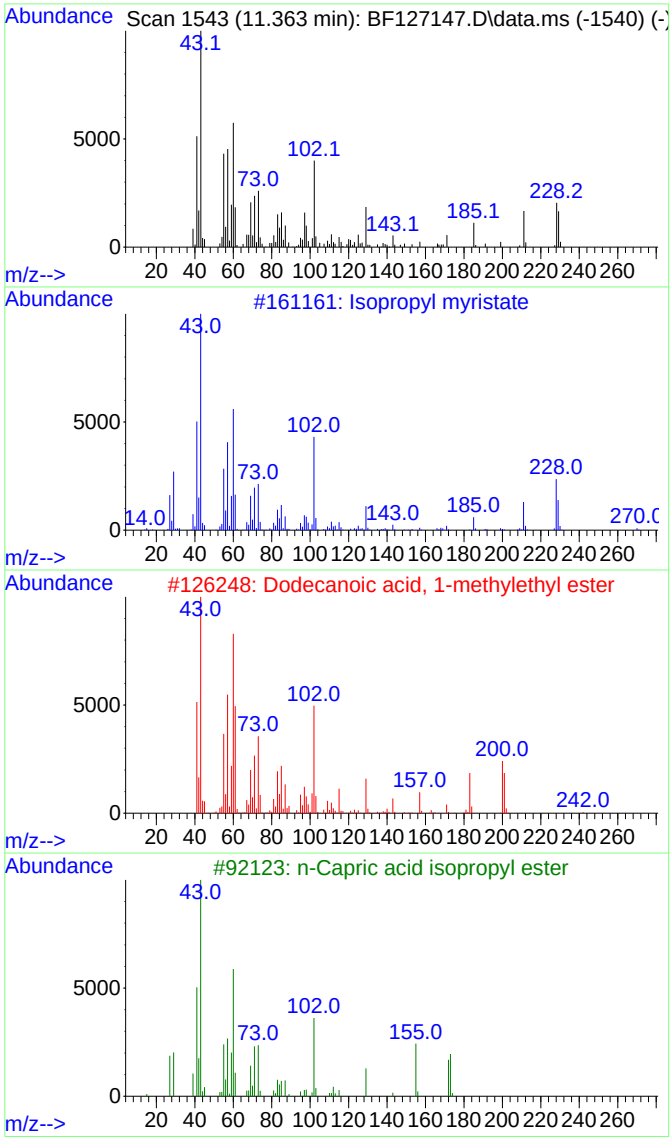
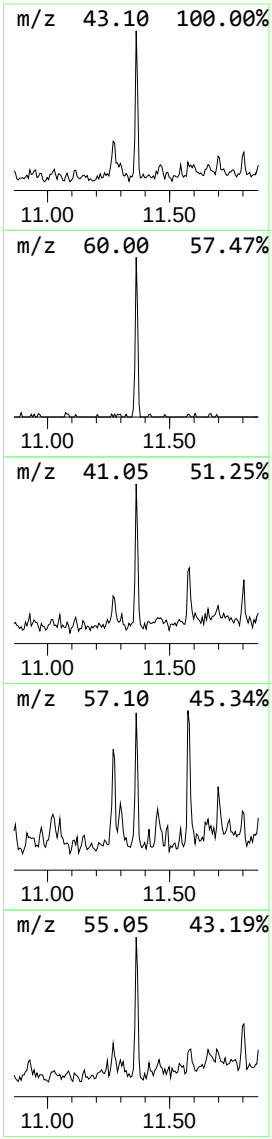
Peak Number 6 Isopropyl myristate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.363	2.74 ng	115756	Phenanthrene-d10	11.422

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl myristate	270	C17H34O2	000110-27-0	83
2	Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	52
3	n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	50
4	Nonanoic acid, 1-methylethyl ester	200	C12H24O2	028267-32-5	42
5	n-Octanoic acid isopropyl ester	186	C11H22O2	005458-59-3	27





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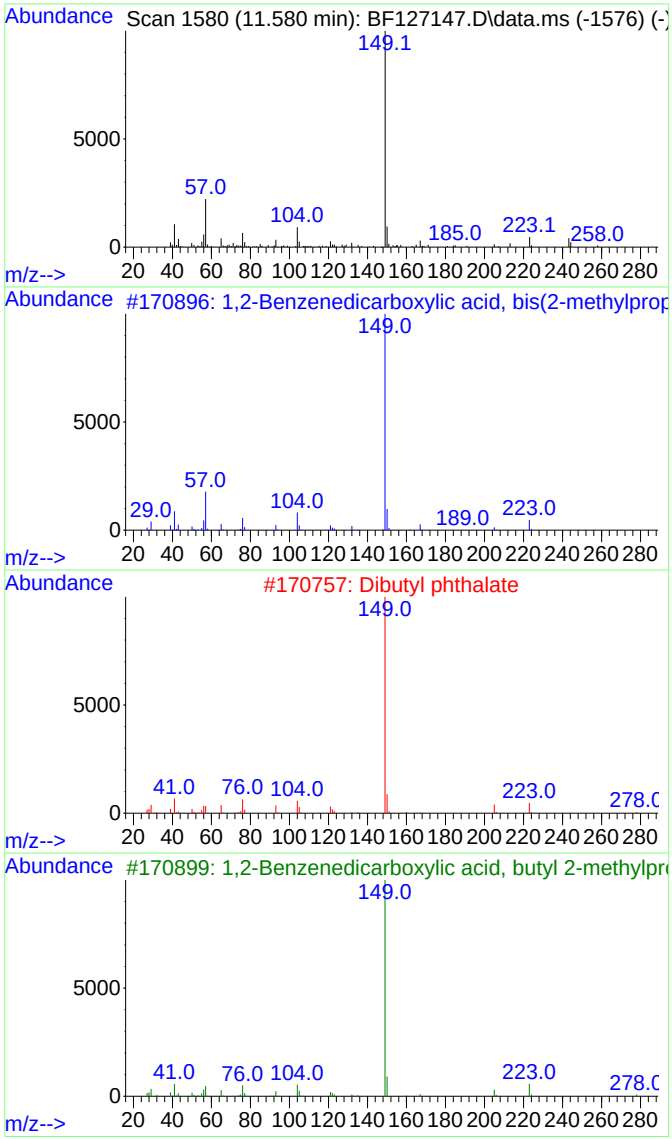
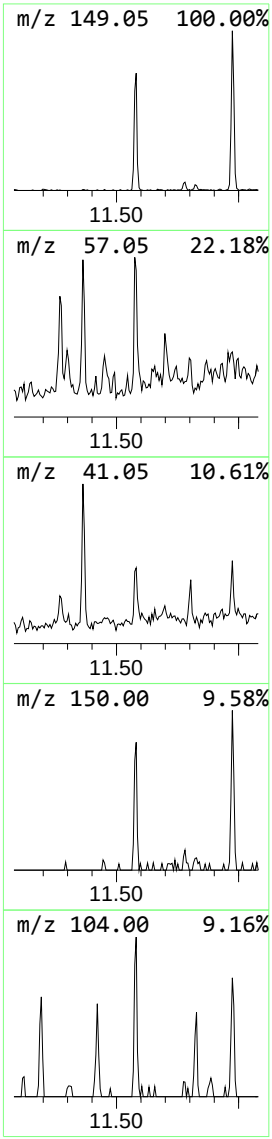
Peak Number 7 1,2-Benzenedicarboxylic aci... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.580	2.77 ng	117029	Phenanthrene-d10	11.422

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	87
2	Dibutyl phthalate	278	C16H22O4	000084-74-2	86
3	1,2-Benzenedicarboxylic acid, bu...	278	C16H22O4	017851-53-5	78
4	Phthalic acid, 5-methylhex-2-yl ...	320	C19H28O4	1000371-09-1	72
5	Phthalic acid, cyclohexylmethyl ...	318	C19H26O4	1000309-08-6	72





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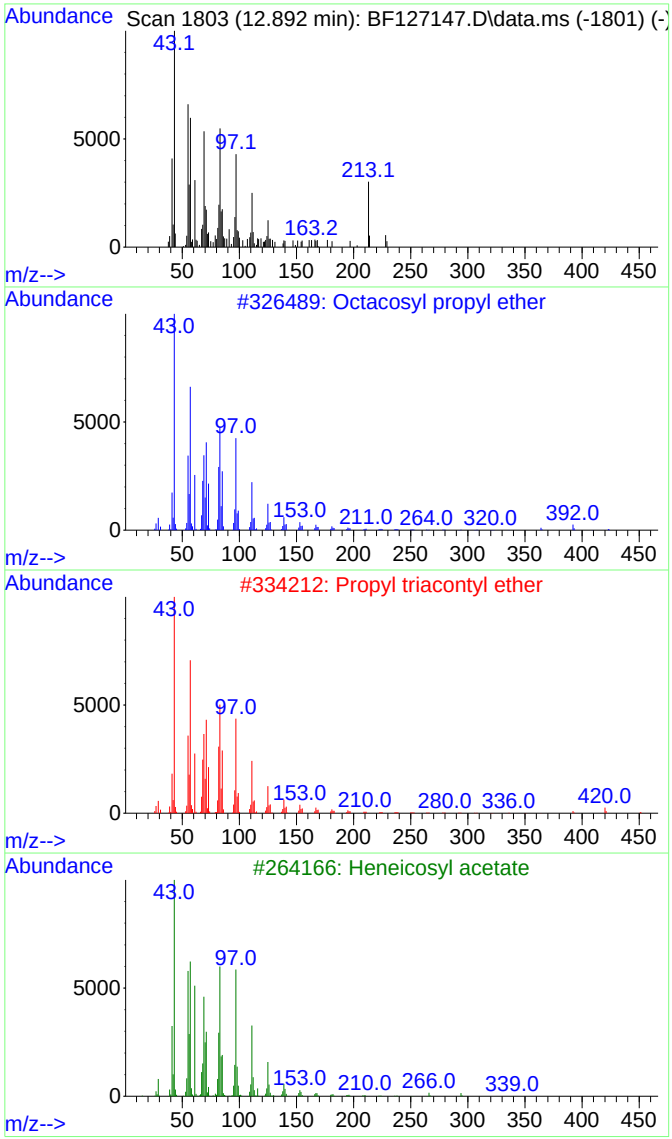
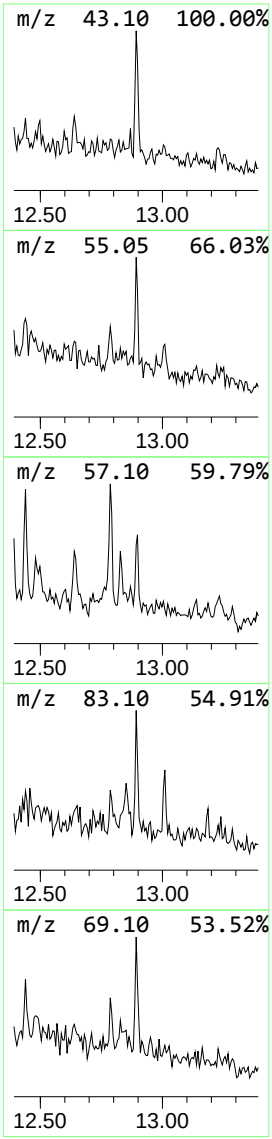
Peak Number 8 Octacosyl propyl ether Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.892	2.87 ng	61155	Chrysene-d12	14.068

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl propyl ether	452	C31H64O	1000406-28-5	72
2	Propyl triacontyl ether	481	C33H68O	1000406-28-6	72
3	Heneicosyl acetate	354	C23H46O2	1000351-77-3	68
4	1-Hexacosene	364	C26H52	018835-33-1	68
5	1-Docosene	308	C22H44	001599-67-3	64





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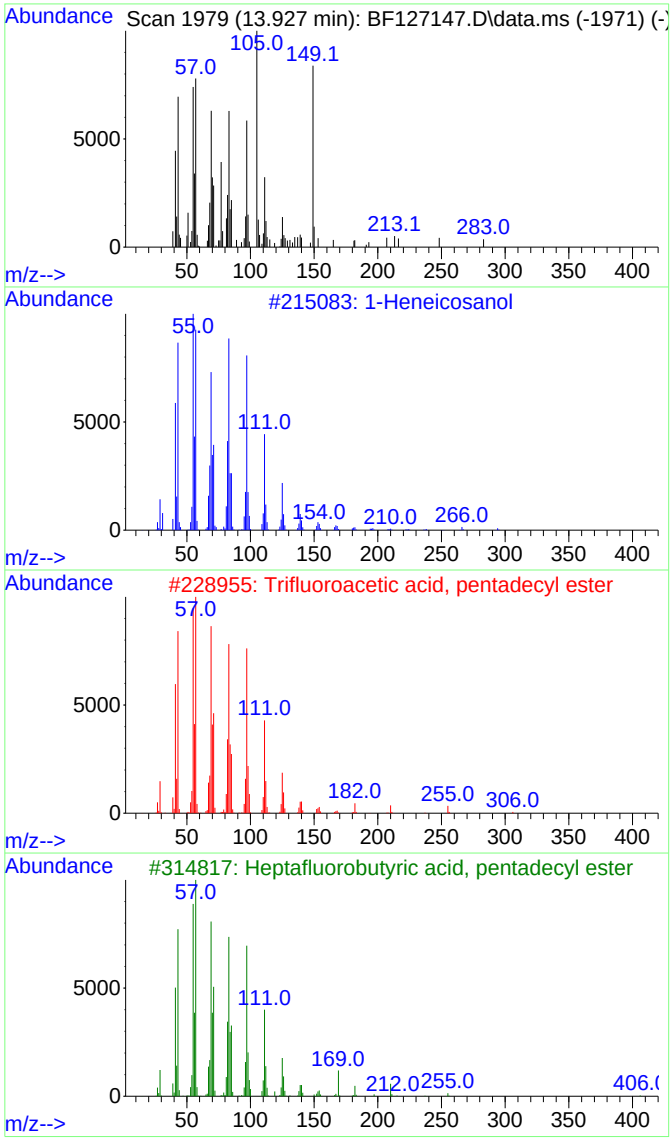
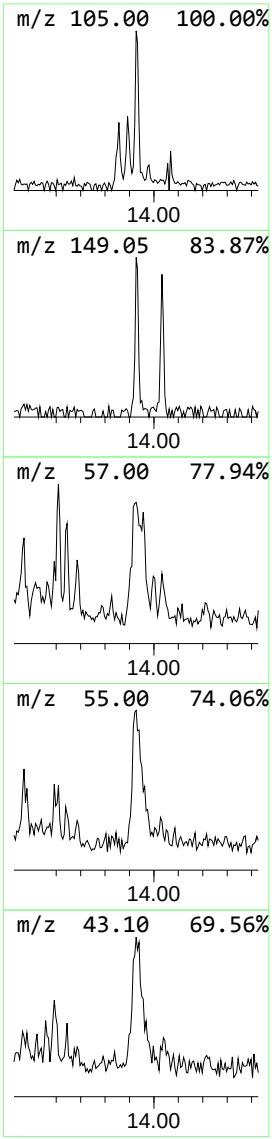
Peak Number 9 1-Heneicosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.927	7.33 ng	156310	Chrysene-d12	14.068

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	84
2	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	84
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	84
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	84
5	Octacosanol	410	C28H58O	000557-61-9	84





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030222\
Data File : BF127147.D
Acq On : 02 Mar 2022 15:12
Operator : CG\JU
Sample : N1725-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-01

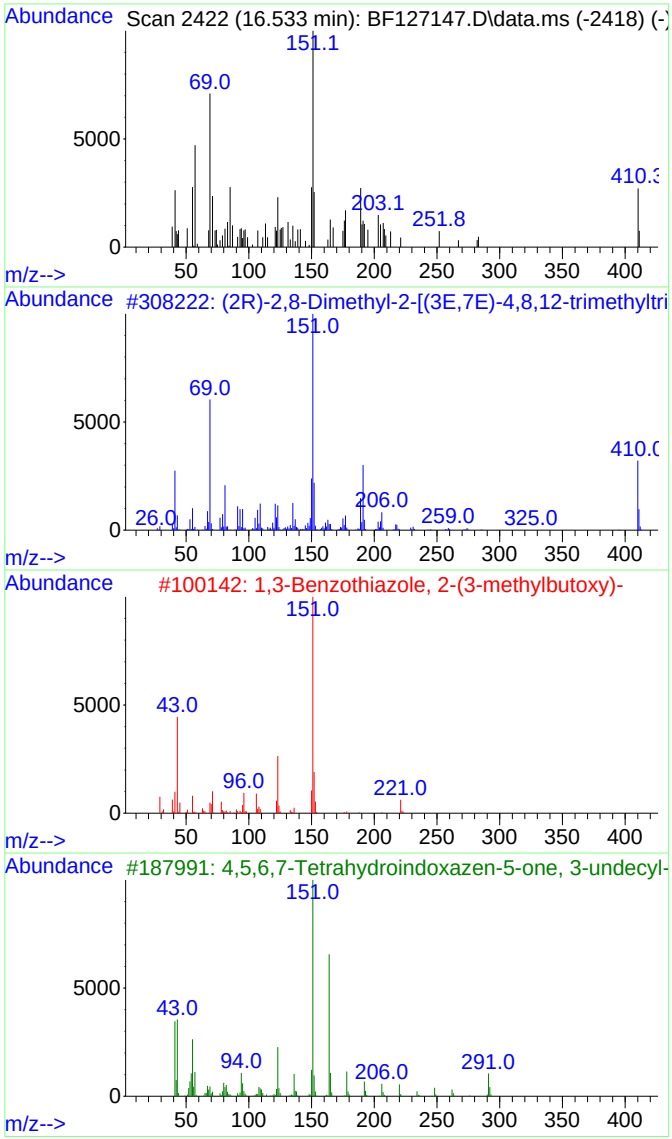
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

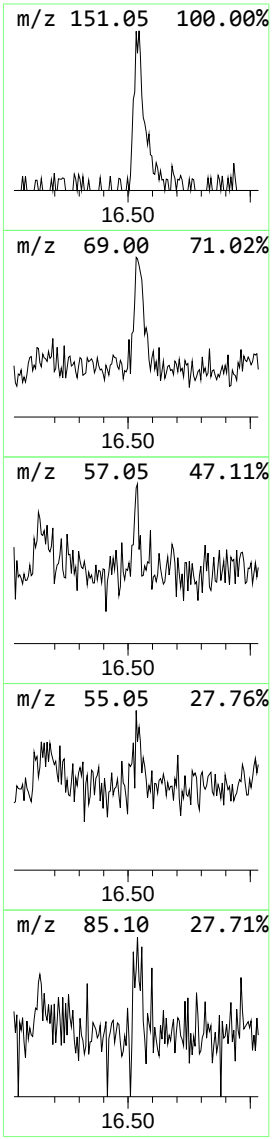
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 (2R)-2,8-Dimethyl-2-[(3E,7E... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.533	2.24 ng	52499	Perylene-d12	15.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(2R)-2,8-Dimethyl-2-[(3E,7E)-4,8...	410	C28H42O2	1000503-47-0	52
2	1,3-Benzothiazole, 2-(3-methylbu...	221	C12H15NOS	1010319-16-3	38
3	4,5,6,7-Tetrahydroindoxazen-5-on...	291	C18H29NO2	123674-79-3	37
4	4-tert-Butylbenzenethiol, S-acetyl-	208	C12H16OS	1000466-98-3	35
5	2-Cyano-3-fluorophenylhydrazine	151	C7H6FN3	1000131-91-9	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030222\
Data File : BF127147.D
Acq On : 02 Mar 2022 15:12
Operator : CG\JU
Sample : N1725-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.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-...	5.110	5.2	ng	147956	1	6.886	573737	20.0
2-Propanol, 1-b...	6.187	3.4	ng	98530	1	6.886	573737	20.0
Ethanol, 2-(2-b...	8.069	3.5	ng	133428	2	8.175	773444	20.0
Nonanoic acid	8.528	10.4	ng	402435	2	8.175	773444	20.0
Cyclohexanamine...	9.586	2.1	ng	91662	3	9.933	853280	20.0
Isopropyl myris...	11.363	2.7	ng	115756	4	11.422	845472	20.0
1,2-Benzenedica...	11.580	2.8	ng	117029	4	11.422	845472	20.0
Octacosyl propy...	12.892	2.9	ng	61155	5	14.068	426236	20.0
1-Heneicosanol	13.927	7.3	ng	156310	5	14.068	426236	20.0
(2R)-2,8-Dimeth...	16.533	2.2	ng	52499	6	15.562	469307	20.0