LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101321\
Data File : BM032489.D
Acq On : 13 Oct 2021 10:59
Operator : CG/JU
Sample : M4170-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P287-DITCH

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-BM100221.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM032489.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.178	392	398	413	rBV	1906481	2599980	27.00%	4.221%
2	6.790	666	672	686	rBV	1004778	1572793	16.33%	2.553%
3	7.601	800	810	818	rBV	838826	1268989	13.18%	2.060%
4	8.754	998	1006	1020	rBV	2538002	4086062	42.44%	6.633%
5	10.166	1240	1246	1259	rBV	683677	1022225	10.62%	1.659%
6	10.389	1277	1284	1298	rBV	1053714	1693308	17.59%	2.749%
7	12.013	1553	1560	1571	rBV2	58981	132367	1.37%	0.215%
8	12.866	1698	1705	1722	rBV	5726906	8505272	88.33%	13.806%
9	14.248	1932	1940	1947	rBV	1416300	2010694	20.88%	3.264%
10	15.677	2161	2183	2187	rBV	135785	722808	7.51%	1.173%
11	15.736	2187	2193	2217	rVB	3880944	6083205	63.18%	9.875%
12	15.913	2218	2223	2228	rBV	154797	239619	2.49%	0.389%
13	16.066	2229	2249	2251	rBV2	246827	1097443	11.40%	1.781%
14	16.342	2274	2296	2327	rBV	1177232	6207441	64.47%	10.076%
15	16.665	2342	2351	2353	rBV	47450	122399	1.27%	0.199%
16	16.977	2398	2404	2410	rBV	1618509	2190691	22.75%	3.556%
17	17.648	2513	2518	2524	rBV	91293	110692	1.15%	0.180%
18	17.877	2544	2557	2582	rBV	1742830	3227889	33.52%	5.240%
19	18.812	2713	2716	2721	rVB	106629	112841	1.17%	0.183%
20	19.148	2767	2773	2792	rBV	1271165	2372856	24.64%	3.852%
21	19.595	2843	2849	2854	rBV	7627159	9628763	100.00%	15.630%
22	20.101	2929	2935	2943	rBV	262344	536330	5.57%	0.871%
23	20.383	2980	2983	2989	rBV	126695	154793	1.61%	0.251%
24	20.848	3058	3062	3064	rBV	324676	429087	4.46%	0.697%
25	21.142	3108	3112	3118	rBV	1866938	2243398	23.30%	3.642%
26	21.524	3173	3177	3184	rBV	307390	488105	5.07%	0.792%
27	22.189	3286	3290	3297	rVB	267470	431752	4.48%	0.701%
28	23.289	3471	3477	3484	rVB2	1335343	2311700	24.01%	3.753%

Sum of corrected areas: 61603502

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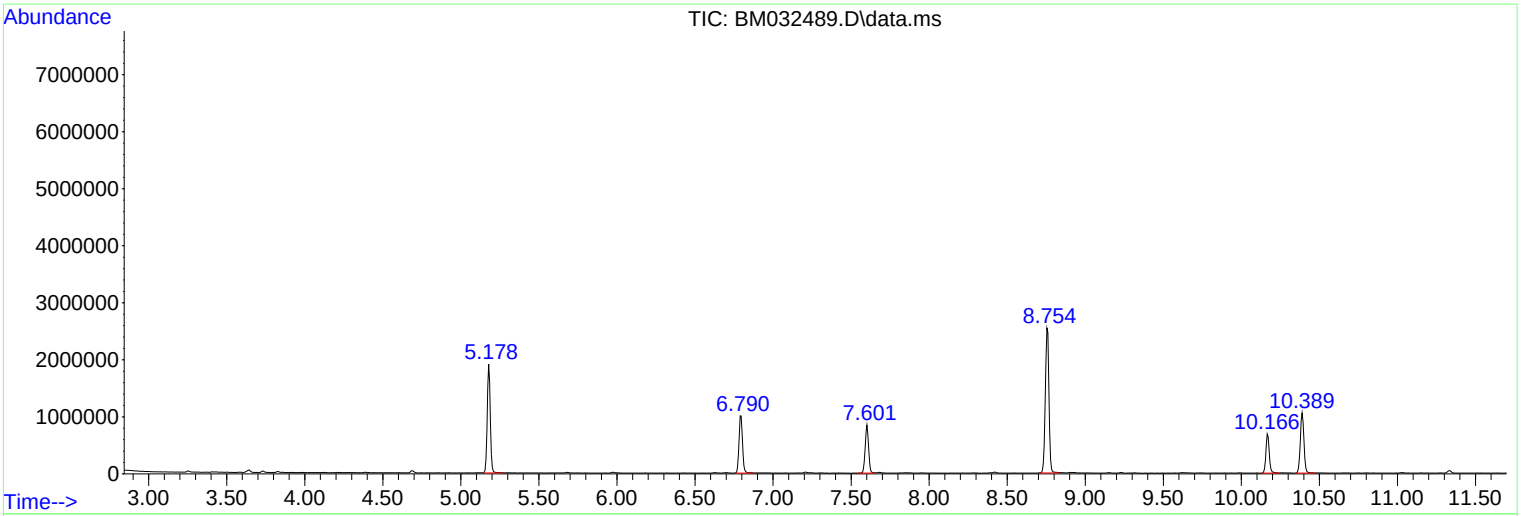
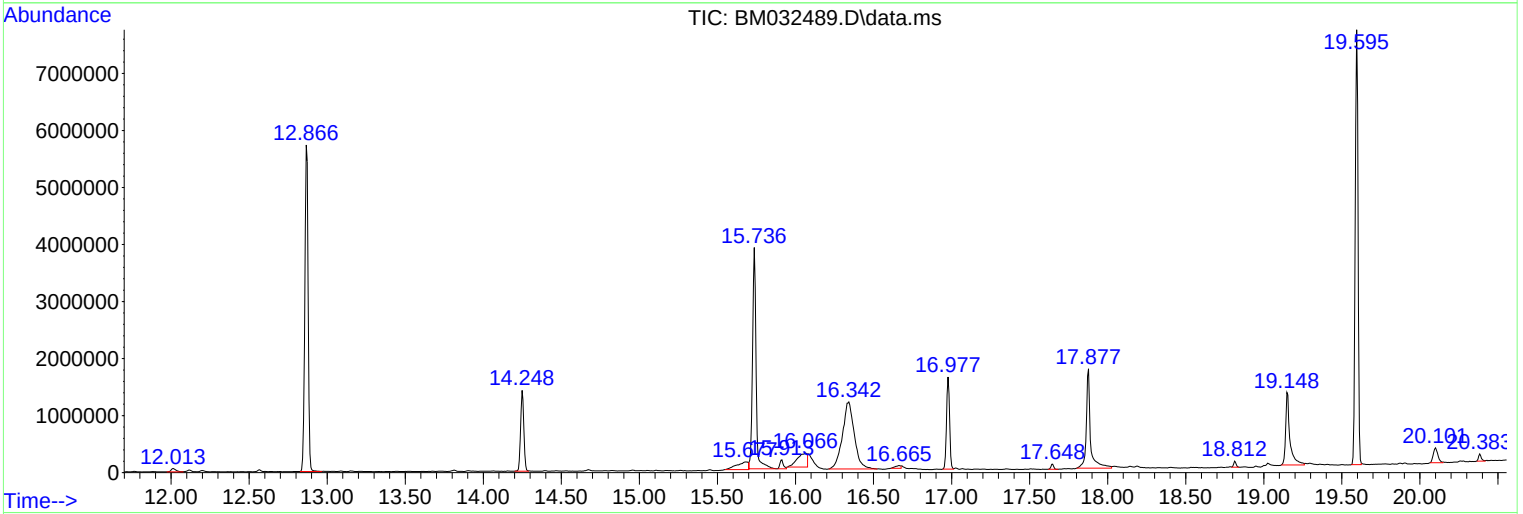
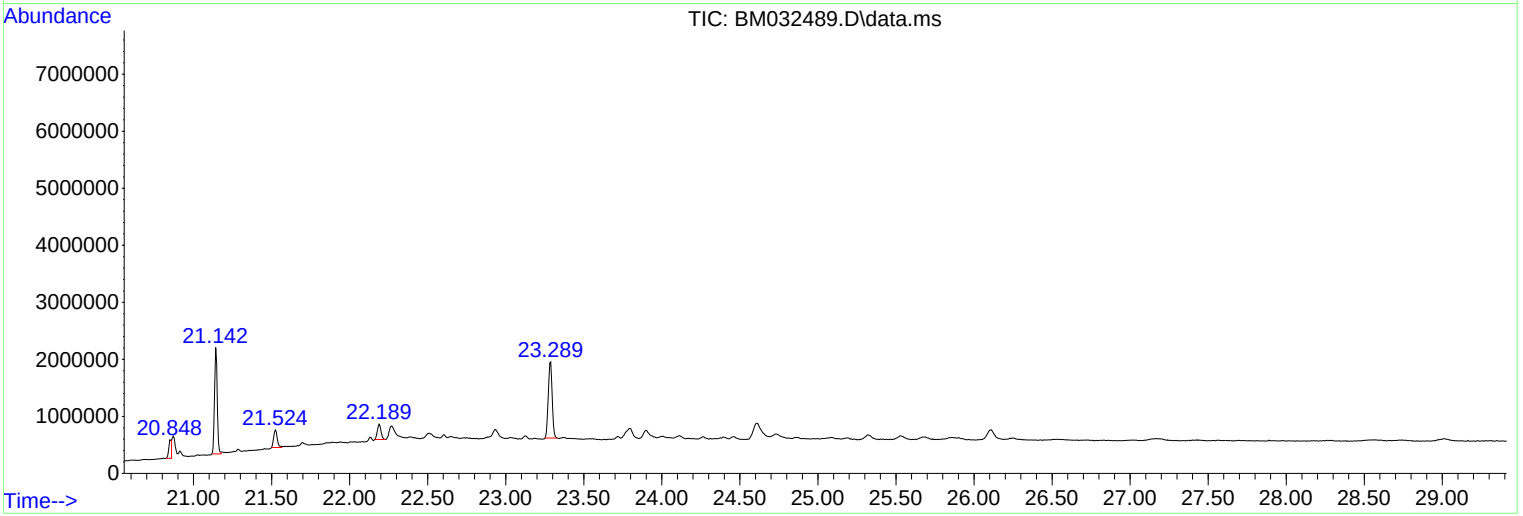
P287-DITCH

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.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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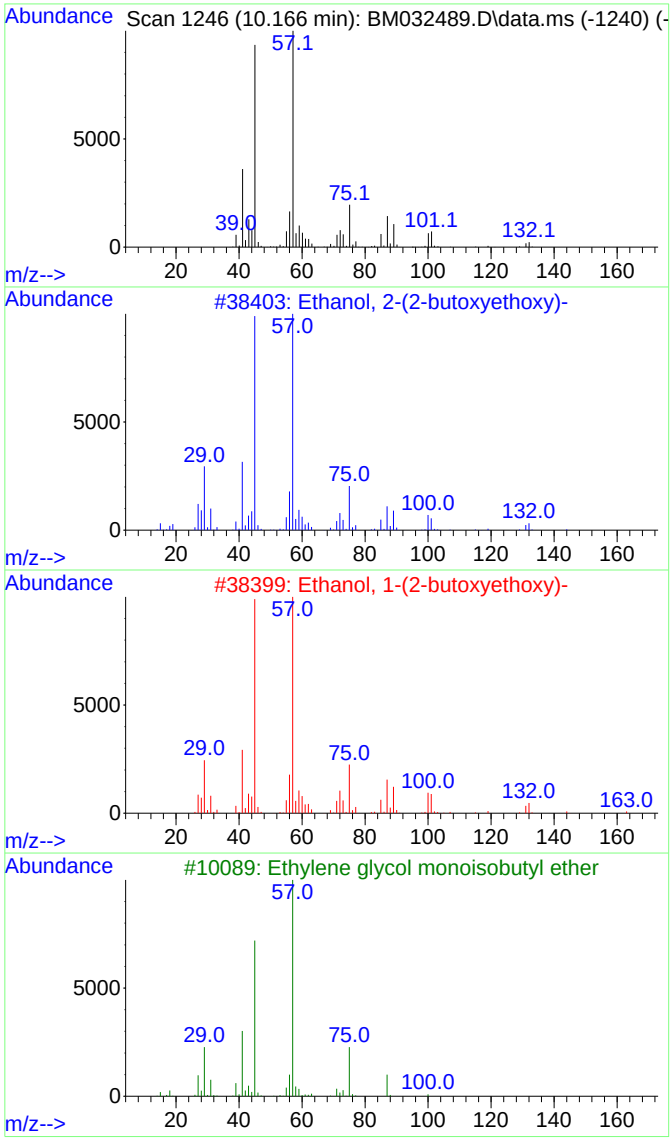
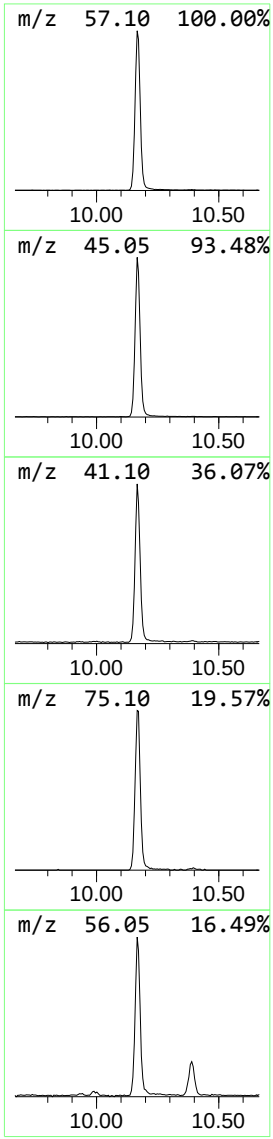
Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.166	12.07 ng	1022230	Naphthalene-d8	10.389

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	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	52





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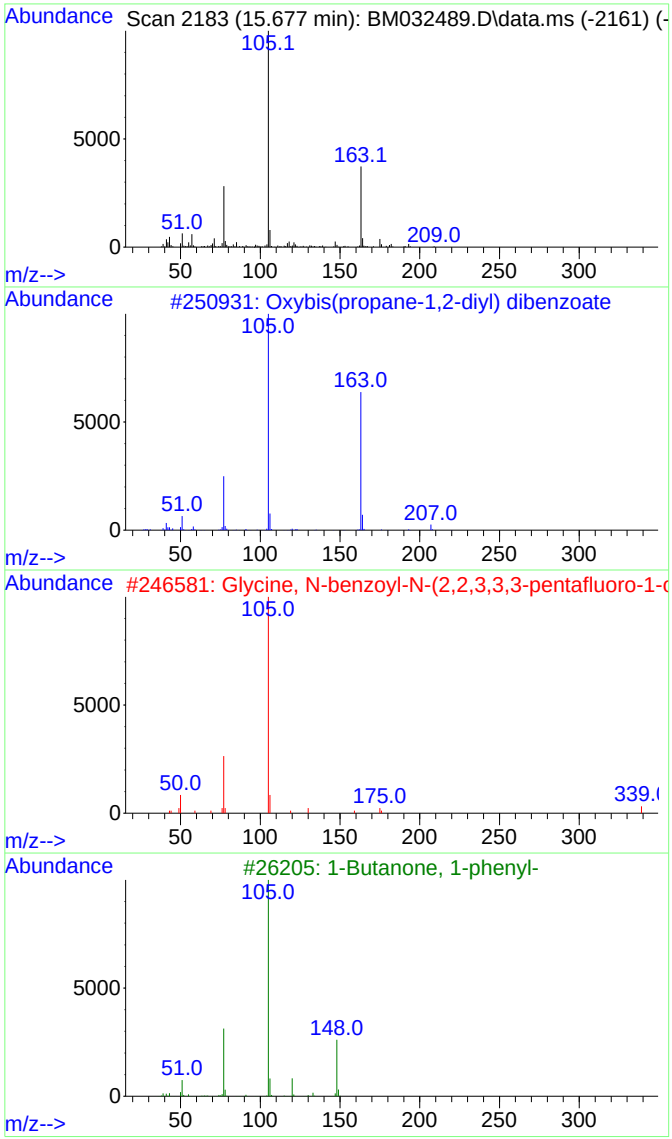
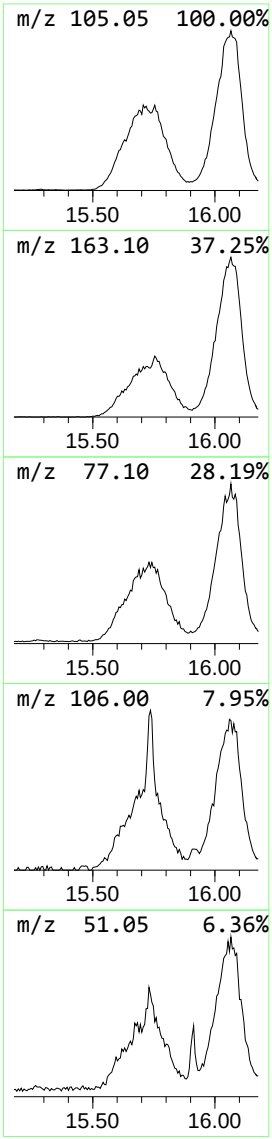
Peak Number 2 Oxybis(propane-1,2-diyl) di... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.677	6.60 ng	722808	Phenanthrene-d10	16.977

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	64
2	Glycine, N-benzoyl-N-(2,2,3,3,3-...	339	C13H10F5NO4	072347-42-3	47
3	1-Butanone, 1-phenyl-	148	C10H12O	000495-40-9	43
4	Phenylglyoxylic acid, neopentyl ...	220	C13H16O3	1000453-45-9	38
5	Phenylglyoxylic acid, pentyl ester	220	C13H16O3	1000453-46-0	38





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ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
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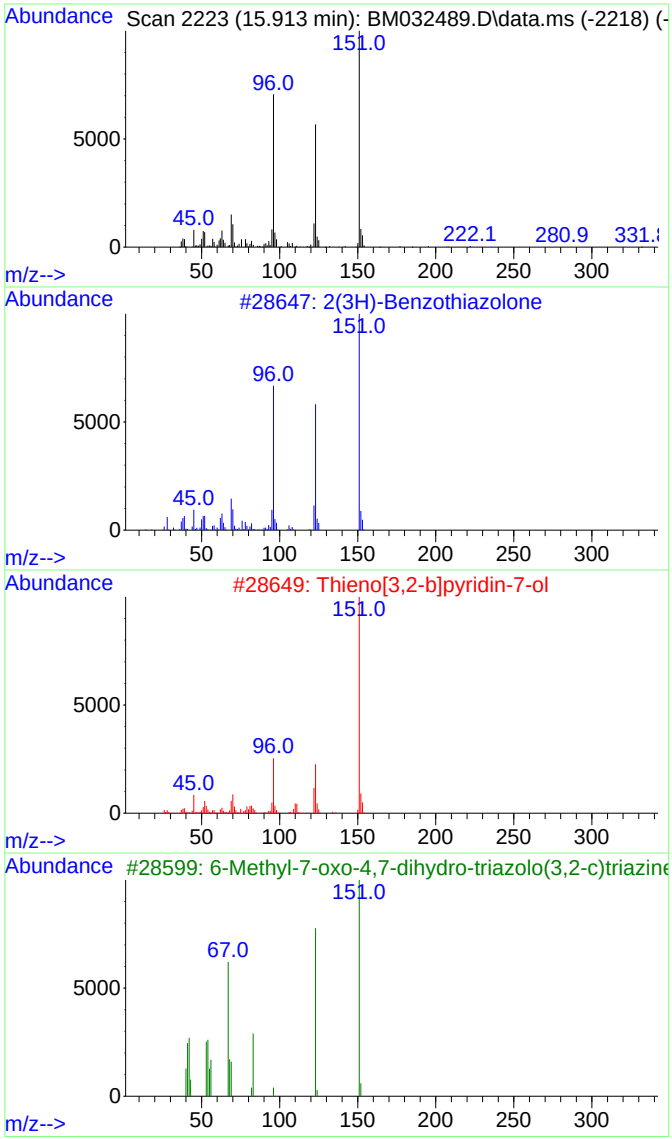
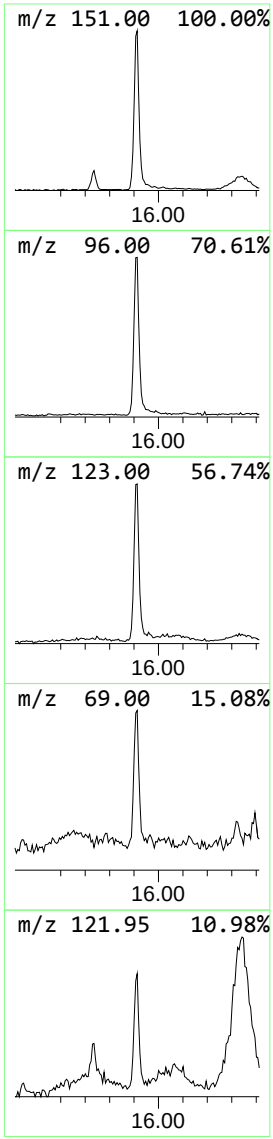
Peak Number 3 2(3H)-Benzothiazolone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.913	2.19 ng	239619	Phenanthrene-d10	16.977

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	96
2	Thieno[3,2-b]pyridin-7-ol	151	C7H5NOS	107818-20-2	64
3	6-Methyl-7-oxo-4,7-dihydro-triaz...	151	C5H5N5O	057250-39-2	50
4	t-Butylhydroquinone	166	C10H14O2	001948-33-0	50
5	1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	45





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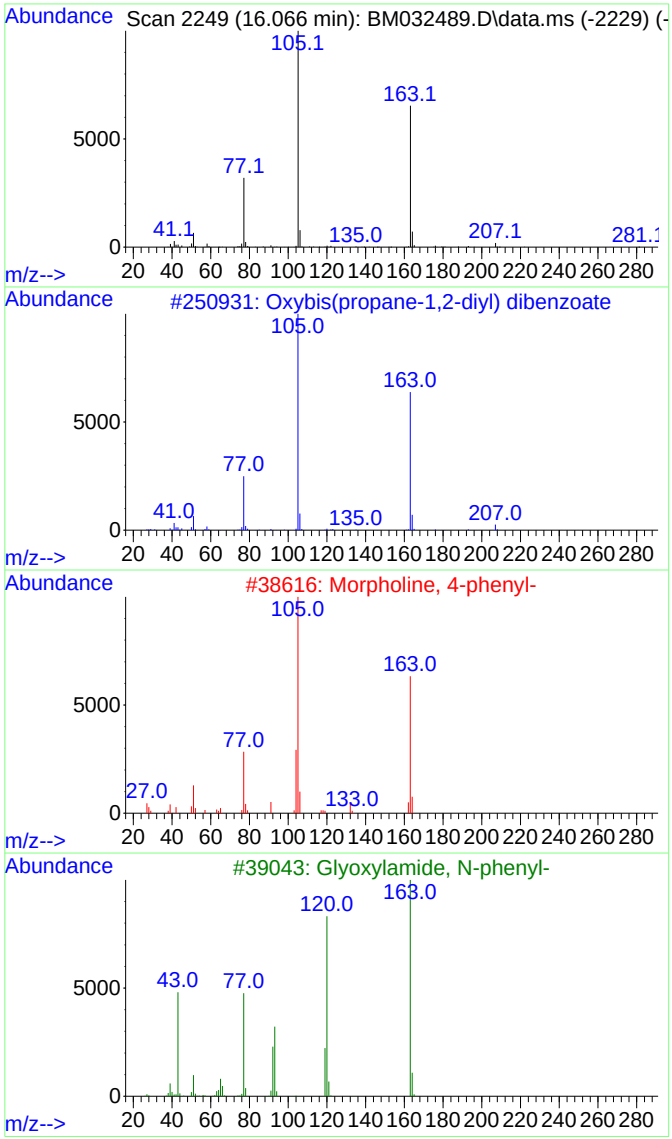
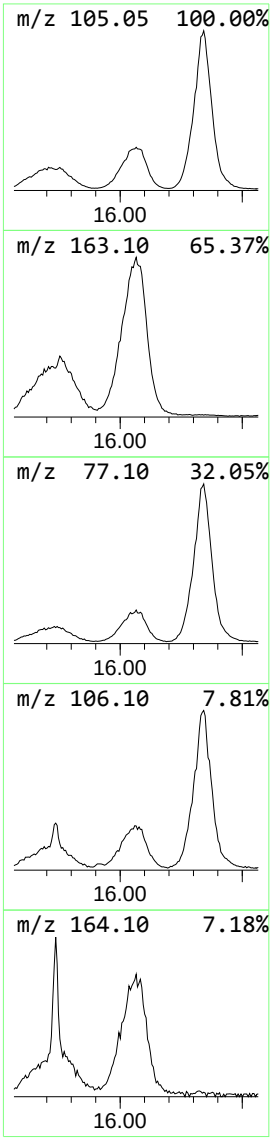
Peak Number 4 Morpholine, 4-phenyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.066	10.02 ng	1097440	Phenanthrene-d10	16.977

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	83
2	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	72
3	Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	50
4	Ethanone, 2-bromo-1,2-diphenyl-	274	C14H11BrO	001484-50-0	38
5	1,3-Benzenediol, monobenzoate	214	C13H10O3	000136-36-7	38





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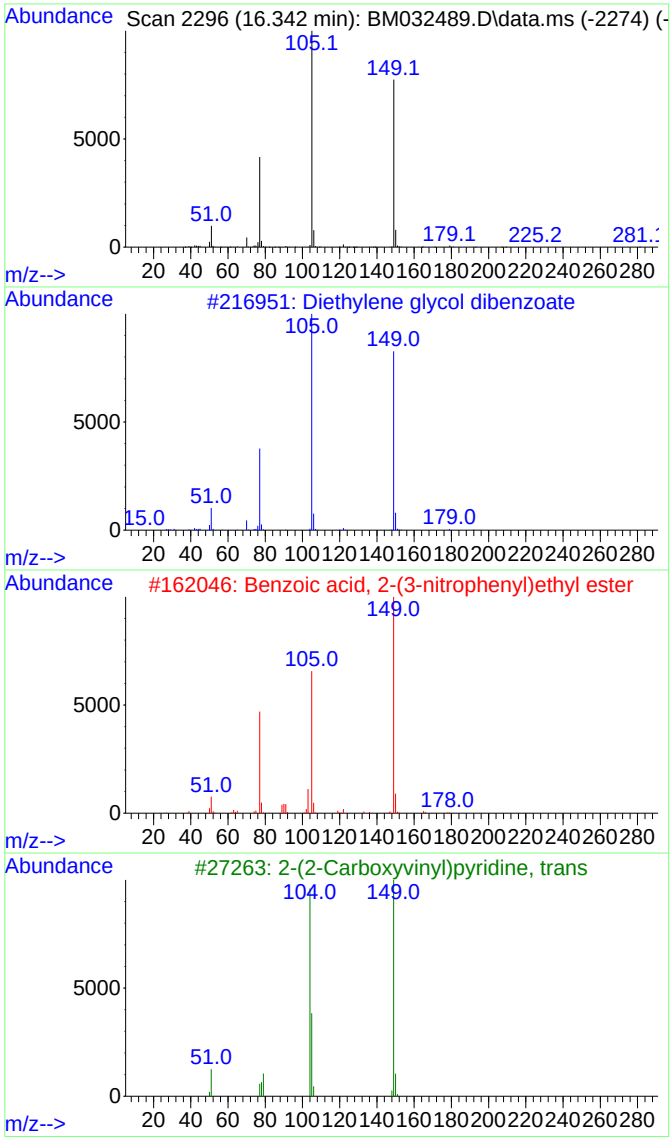
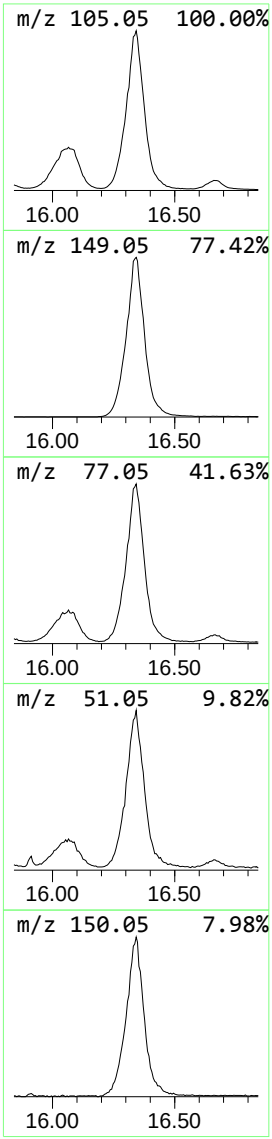
Peak Number 5 Diethylene glycol dibenzoate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.342	56.67 ng	6207440	Phenanthrene-d10	16.977

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	91
2	Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	72
3	2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	49
4	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	47
5	2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	43





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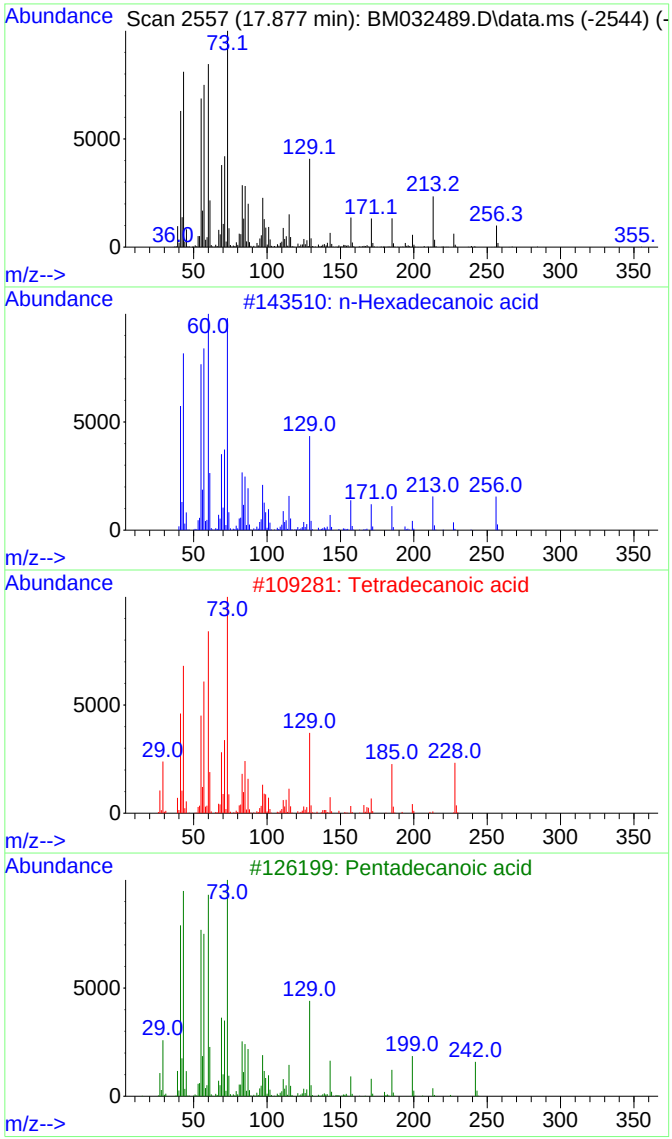
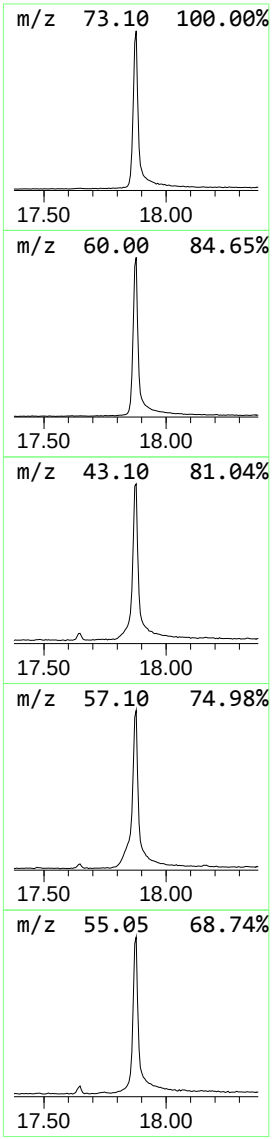
Peak Number 6 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.877	29.47 ng	3227890	Phenanthrene-d10	16.977

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tridecanoic acid	214	C13H26O2	000638-53-9	91
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





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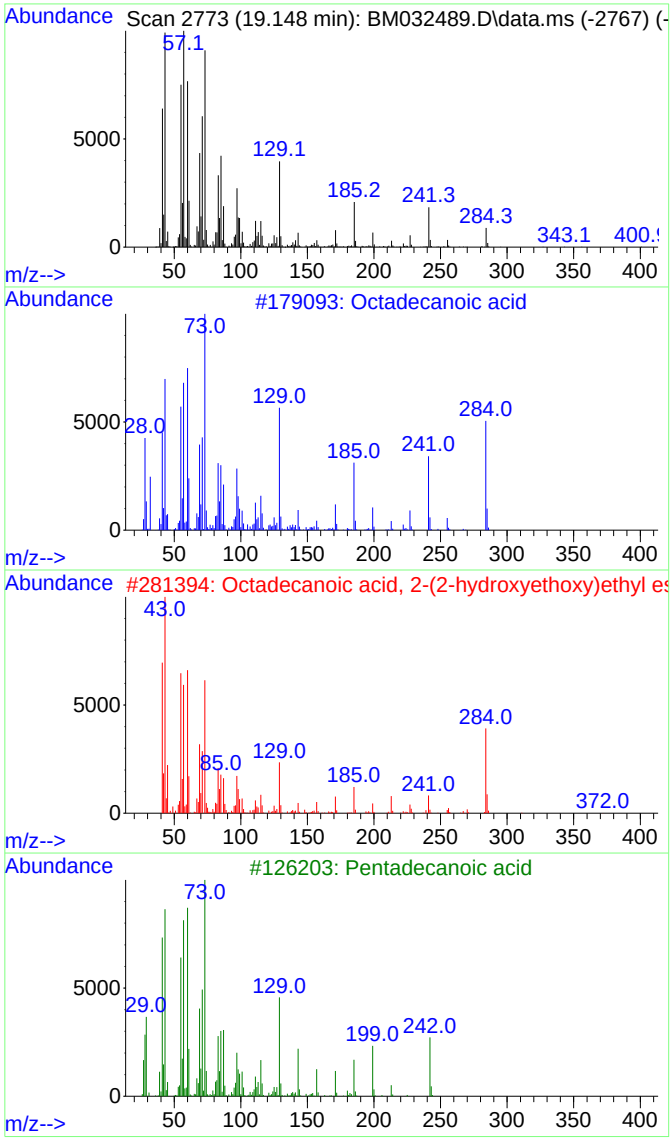
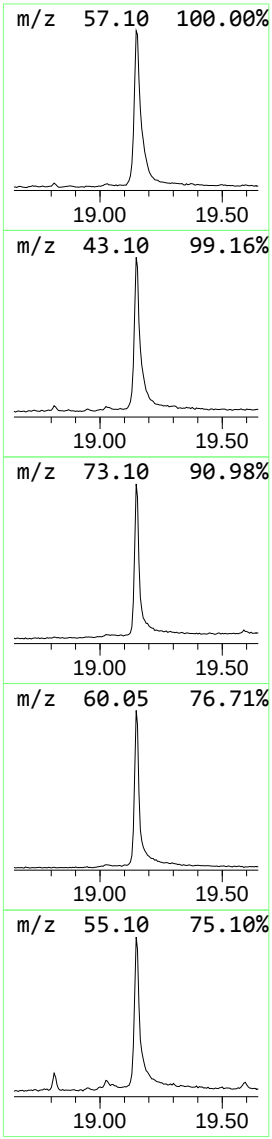
Peak Number 7 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.148	21.15 ng	2372860	Chrysene-d12	21.142

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	83
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	43





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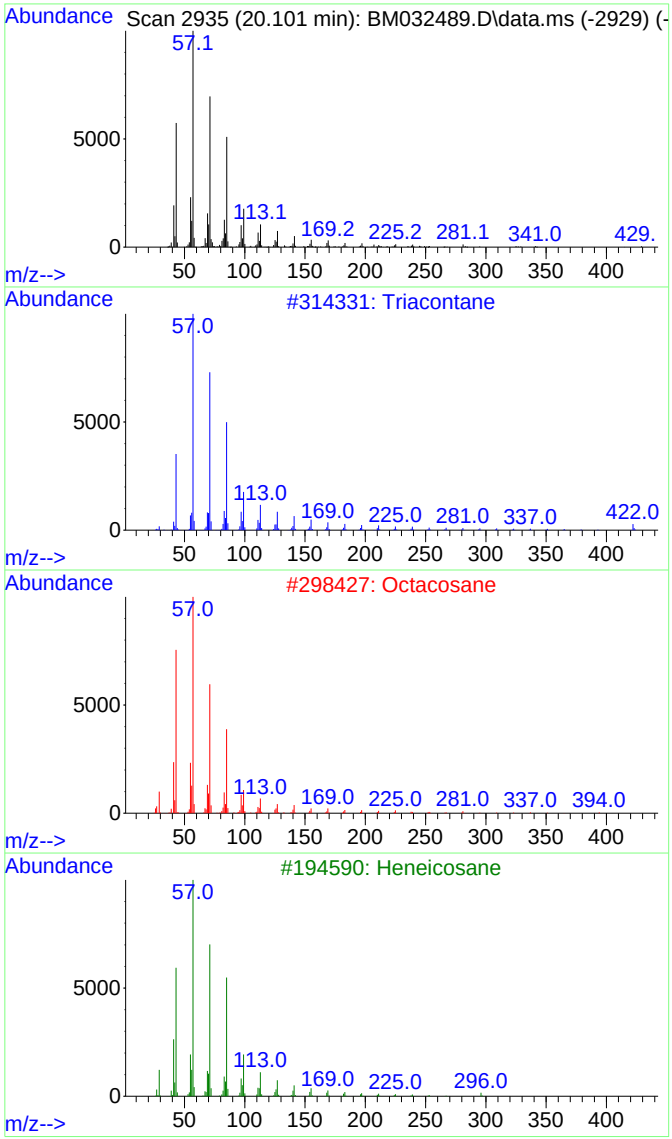
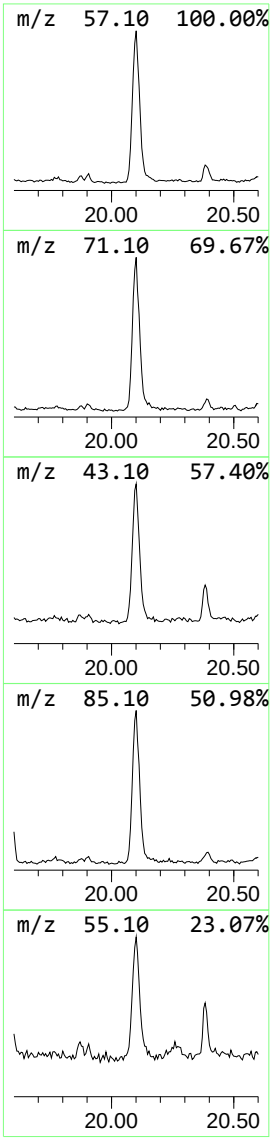
Peak Number 8 Triacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.101	4.78 ng	536330	Chrysene-d12	21.142

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Triacontane, 1-iodo-	548	C30H61I	1000406-32-3	91
5	Docosane, 11-butyl-	366	C26H54	013475-76-8	91





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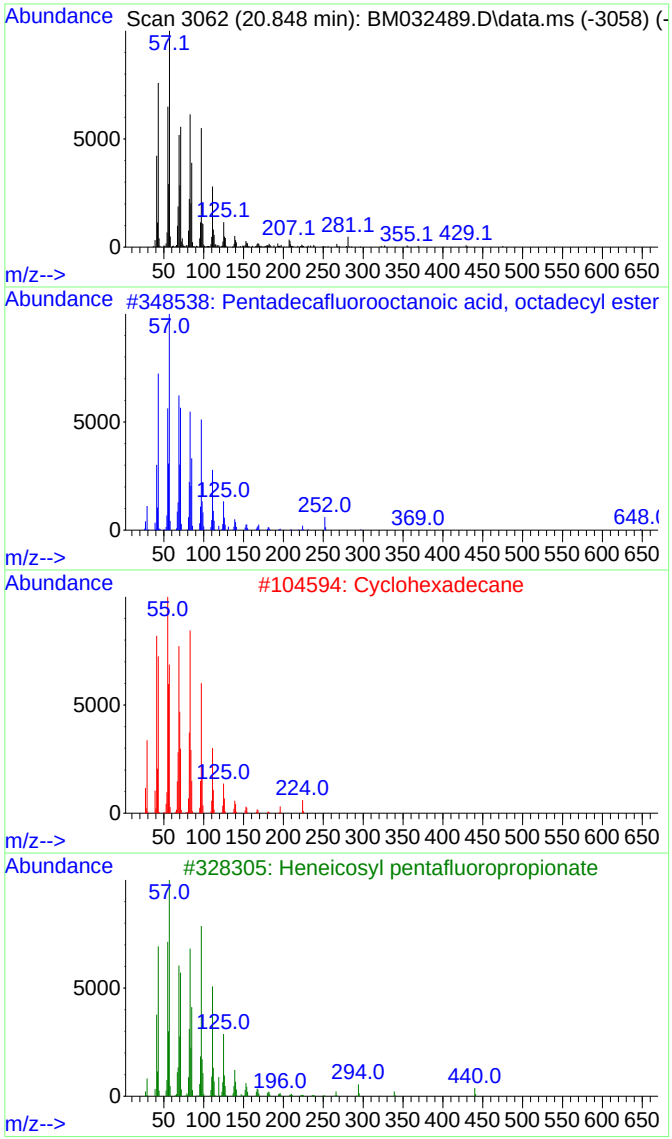
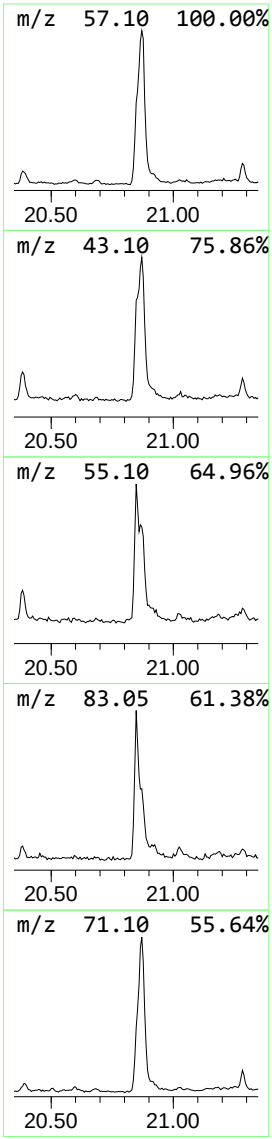
Peak Number 9 Pentadecafluorooctanoic aci... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.848	3.83 ng	429087	Chrysene-d12	21.142

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2	Cyclohexadecane	224	C16H32	000295-65-8	92
3	Heneicosyl pentafluoropropionate	458	C24H43F5O2	1000351-81-1	91
4	Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	91
5	Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	91





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Acq On : 13 Oct 2021 10:59
Operator : CG/JU
Sample : M4170-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P287-DITCH

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.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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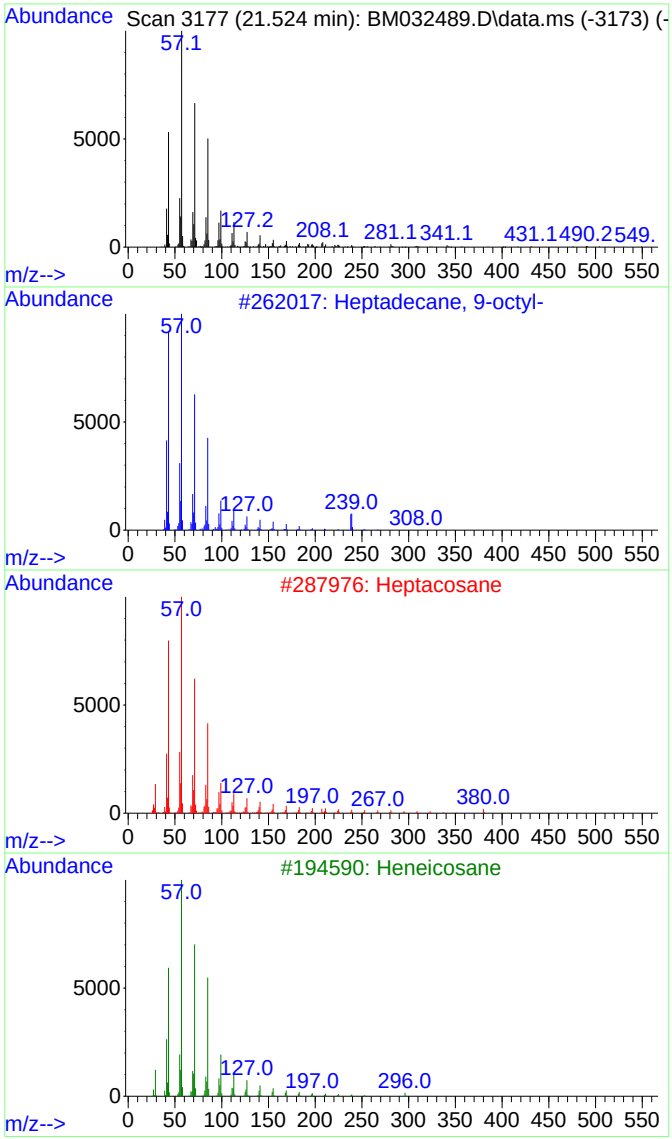
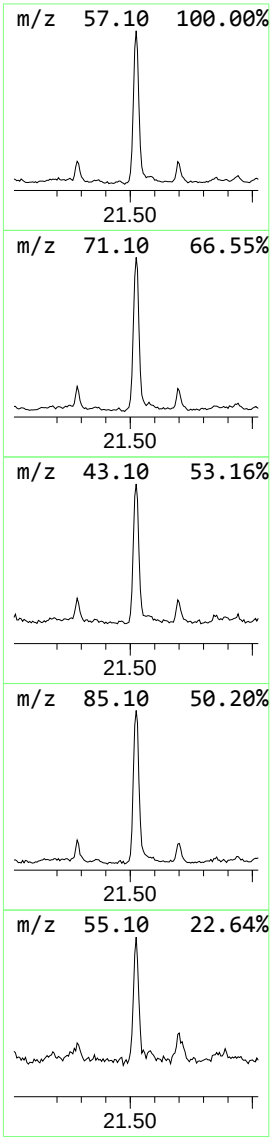
Peak Number 10 Heptadecane, 9-octyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.524	4.35 ng	488105	Chrysene-d12	21.142

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
2	Heptacosane	380	C27H56	000593-49-7	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	Octacosane	394	C28H58	000630-02-4	90
5	Octacosane, 2-methyl-	408	C29H60	001560-98-1	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101321\
Data File : BM032489.D
Acq On : 13 Oct 2021 10:59
Operator : CG/JU
Sample : M4170-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P287-DITCH

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.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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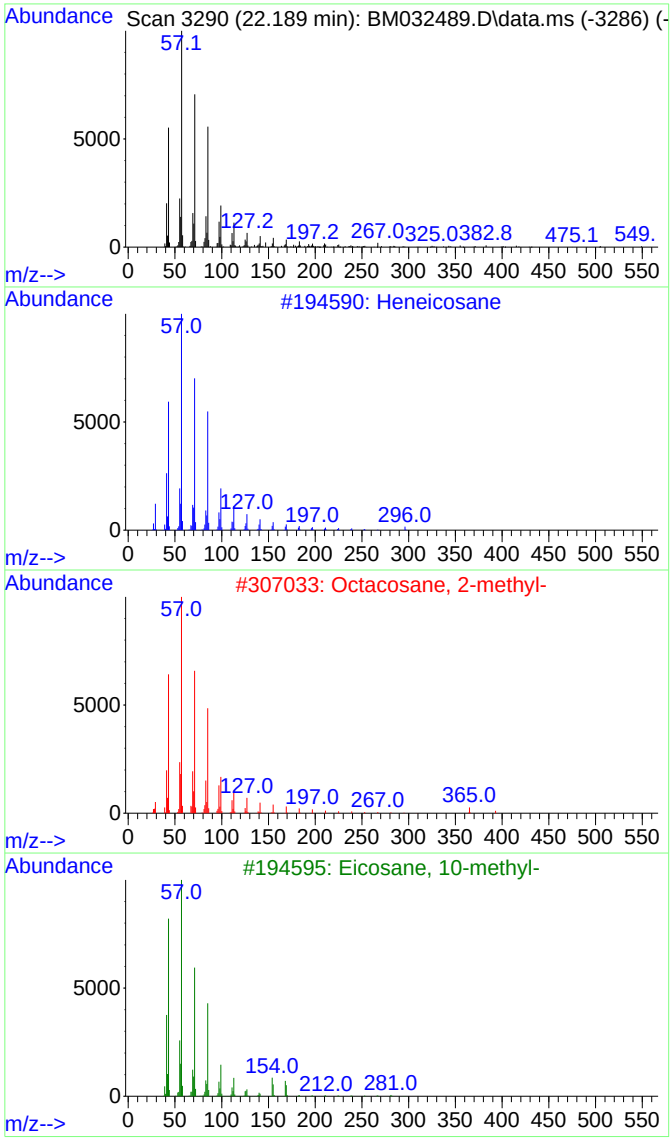
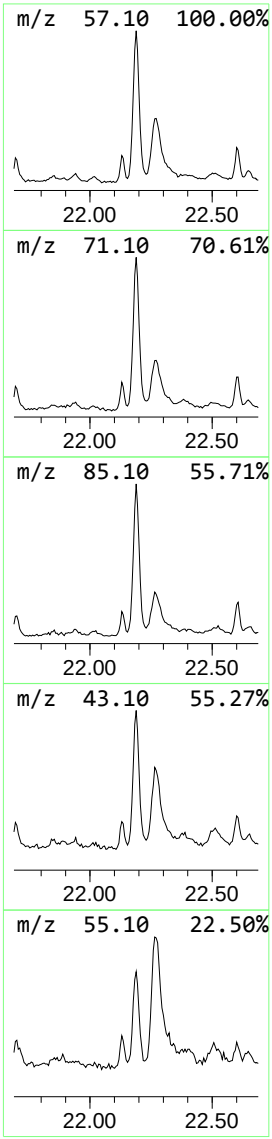
Peak Number 11 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.189	3.85 ng	431752	Chrysene-d12	21.142

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
3	Eicosane, 10-methyl-	296	C21H44	054833-23-7	90
4	Tetracosane	338	C24H50	000646-31-1	87
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101321\
Data File : BM032489.D
Acq On : 13 Oct 2021 10:59
Operator : CG/JU
Sample : M4170-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P287-DITCH

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.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
Ethanol, 2-(2-b...	10.166	12.1	ng	1022230	2	10.389	1693310	20.0
Oxybis(propane-...	15.677	6.6	ng	722808	4	16.977	2190690	20.0
2(3H)-Benzothia...	15.913	2.2	ng	239619	4	16.977	2190690	20.0
Morpholine, 4-p...	16.066	10.0	ng	1097440	4	16.977	2190690	20.0
Diethylene glyc...	16.342	56.7	ng	6207440	4	16.977	2190690	20.0
n-Hexadecanoic ...	17.877	29.5	ng	3227890	4	16.977	2190690	20.0
Octadecanoic acid	19.148	21.1	ng	2372860	5	21.142	2243400	20.0
Triacontane	20.101	4.8	ng	536330	5	21.142	2243400	20.0
Pentadecafluoro...	20.848	3.8	ng	429087	5	21.142	2243400	20.0
Heptadecane, 9-...	21.524	4.3	ng	488105	5	21.142	2243400	20.0
Heneicosane	22.189	3.9	ng	431752	5	21.142	2243400	20.0