LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120221\
Data File : BP008198.D
Acq On : 02 Dec 2021 18:52
Operator : CG/JU
Sample : M4877-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PL-2-120121

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_P\Methods\8270E-BP112521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008198.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.046	8	10	19	rVB2	37466	55641	1.40%	0.208%
2	4.922	323	329	340	rBV	219492	306166	7.69%	1.144%
3	5.387	402	408	421	rBV	1256631	1885322	47.38%	7.044%
4	6.981	671	679	694	rBV	1178972	1966746	49.43%	7.348%
5	7.793	809	817	825	rBV	325947	522823	13.14%	1.953%
6	8.957	1006	1015	1034	rBV	740263	1279070	32.15%	4.779%
7	10.393	1253	1259	1266	rBV2	22568	46677	1.17%	0.174%
8	10.593	1284	1293	1302	rBV	413017	706374	17.75%	2.639%
9	13.063	1706	1713	1726	rBV	1825895	2691079	67.63%	10.054%
10	14.104	1884	1890	1897	rBV2	24332	50390	1.27%	0.188%
11	14.439	1941	1947	1956	rBV	594567	920390	23.13%	3.439%
12	15.257	2080	2086	2091	rBV2	24110	57664	1.45%	0.215%
13	15.939	2196	2202	2211	rBV	1386693	2126171	53.44%	7.943%
14	17.133	2398	2405	2410	rBV	50693	80947	2.03%	0.302%
15	17.204	2410	2417	2422	rBV	757420	1121265	28.18%	4.189%
16	17.504	2463	2468	2472	rBV2	23241	41796	1.05%	0.156%
17	17.604	2479	2485	2492	rBV2	17390	47503	1.19%	0.177%
18	18.045	2556	2560	2566	rVV	135382	202476	5.09%	0.756%
19	18.104	2566	2570	2577	rVV	266627	387018	9.73%	1.446%
20	18.392	2615	2619	2622	rBV2	30149	44177	1.11%	0.165%
21	18.522	2637	2641	2645	rVB3	35290	40871	1.03%	0.153%
22	19.227	2757	2761	2768	rBV	91619	143149	3.60%	0.535%
23	19.345	2778	2781	2788	rVB4	57060	85121	2.14%	0.318%
24	19.574	2817	2820	2829	rVB	60148	87813	2.21%	0.328%
25	19.774	2849	2854	2861	rBV	3135251	3978976	100.00%	14.865%
26	20.057	2899	2902	2905	rBV4	48808	78840	1.98%	0.295%
27	21.027	3063	3067	3072	rBV	451900	668823	16.81%	2.499%
28	21.310	3110	3115	3119	rBV	987378	1329269	33.41%	4.966%
29	21.945	3217	3223	3231	rBV	470482	841345	21.14%	3.143%
30	22.668	3342	3346	3352	rVB2	425598	626577	15.75%	2.341%
31	22.980	3394	3399	3403	rBV	436357	683798	17.19%	2.555%
32	23.033	3403	3408	3417	rVB2	718389	1386336	34.84%	5.179%
33	23.704	3516	3522	3529	rVB	619910	1314432	33.03%	4.911%
34	24.333	3624	3629	3639	rVB	440408	961588	24.17%	3.592%

Sum of corrected areas: 26766633

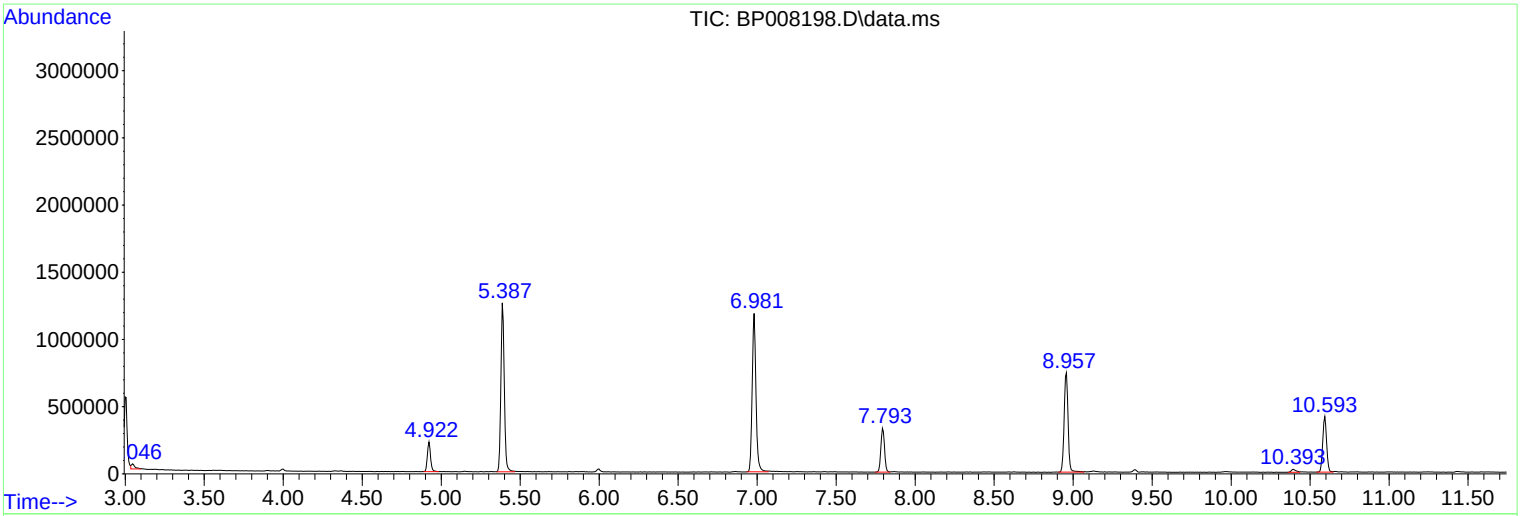
Instrument :
BNA_P
ClientSampleId :
PL-2-120121

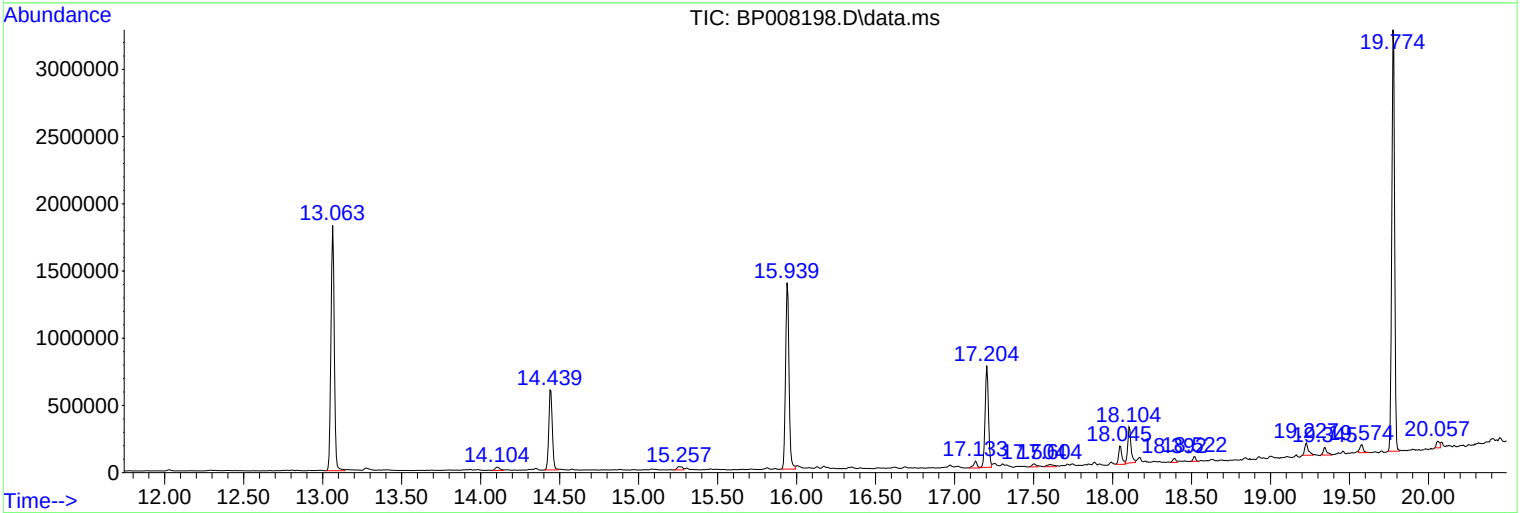
Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120221\
Data File : BP008198.D
Acq On : 02 Dec 2021 18:52
Operator : CG/JU
Sample : M4877-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

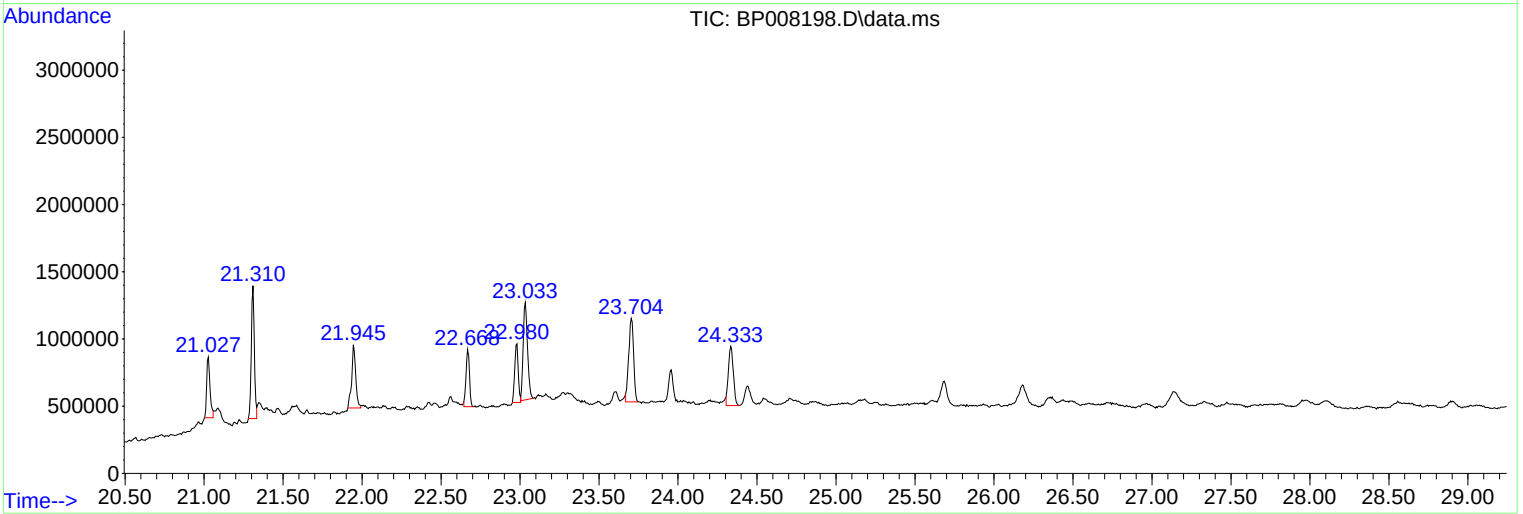
Instrument :
BNA_P
ClientSampleId :
PL-2-120121

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.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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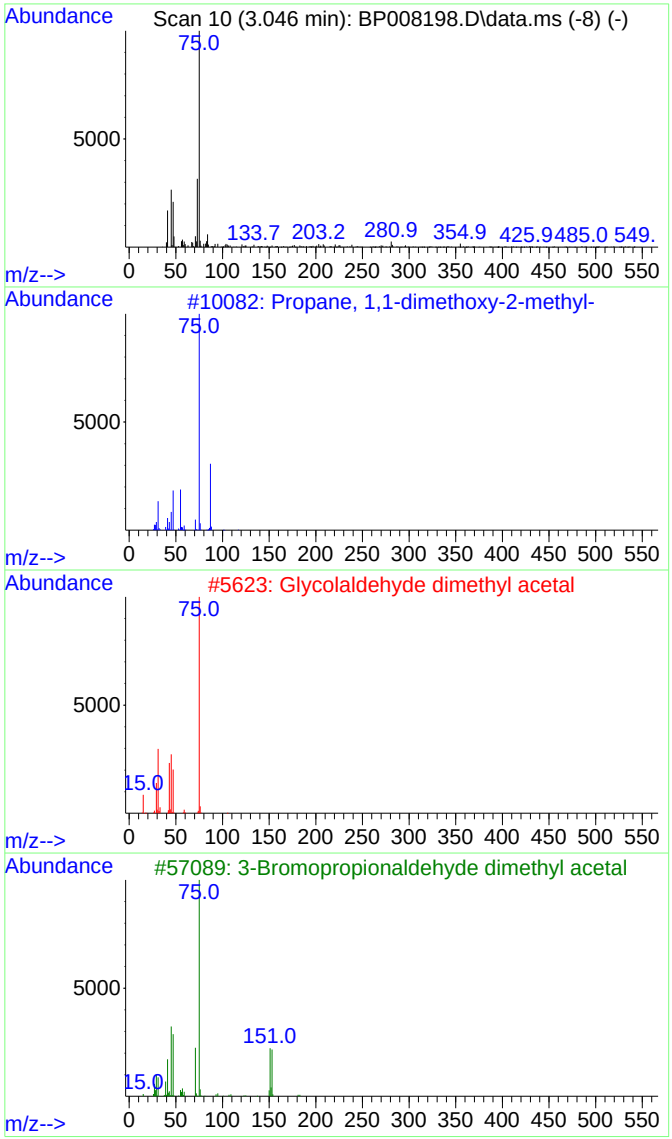
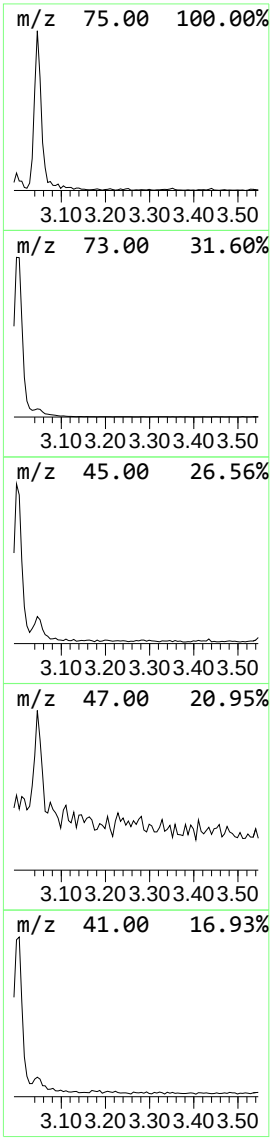
****
Peak Number 1 Propane, 1,1-dimethoxy-2-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.046	2.13 ng	55641	1,4-Dichlorobenzene-d4	7.793

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-2-methyl-	118	C6H14O2	041632-89-7	50
2	Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	45
3	3-Bromopropionaldehyde dimethyl ...	182	C5H11BrO2	036255-44-4	45
4	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	36
5	2-Propanol, 1,1-dimethoxy-, acetate	162	C7H14O4	074495-37-7	33





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Operator : CG/JU
Sample : M4877-01
Misc :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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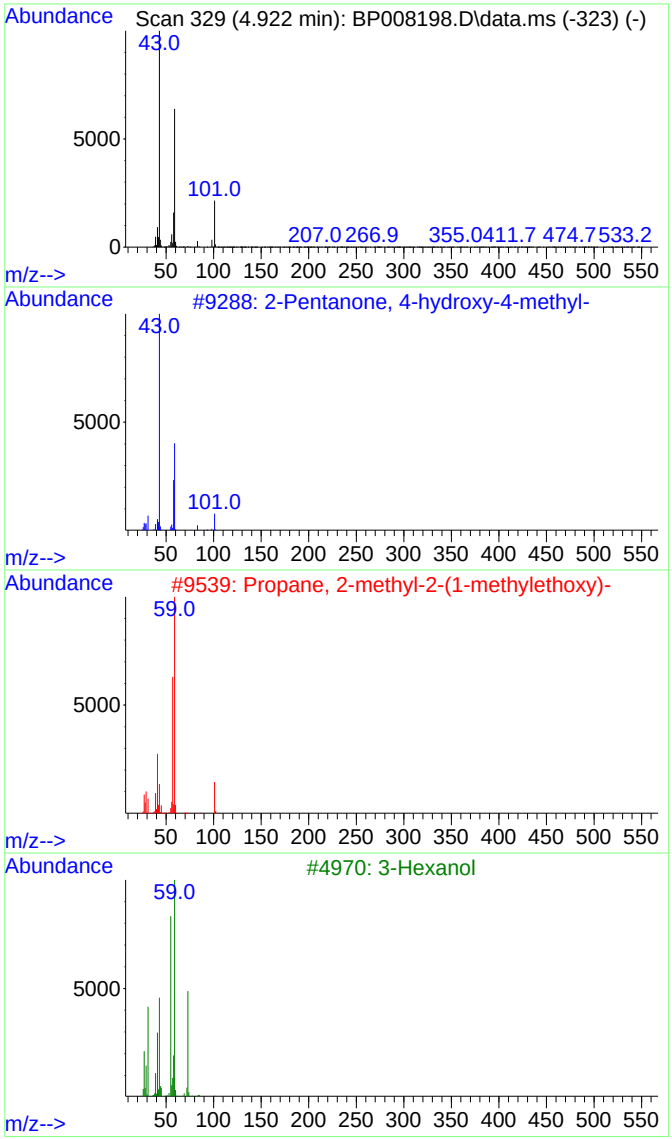
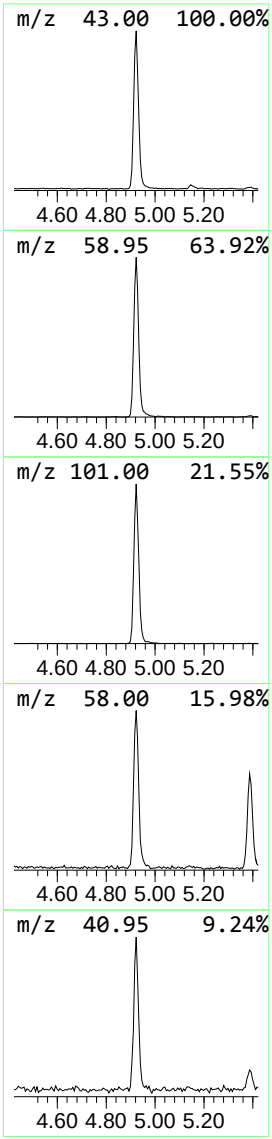
****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.922	11.71 ng	306166	1,4-Dichlorobenzene-d4	7.793

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	50
3	3-Hexanol	102	C6H14O	000623-37-0	33
4	3-Octanol	130	C8H18O	000589-98-0	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
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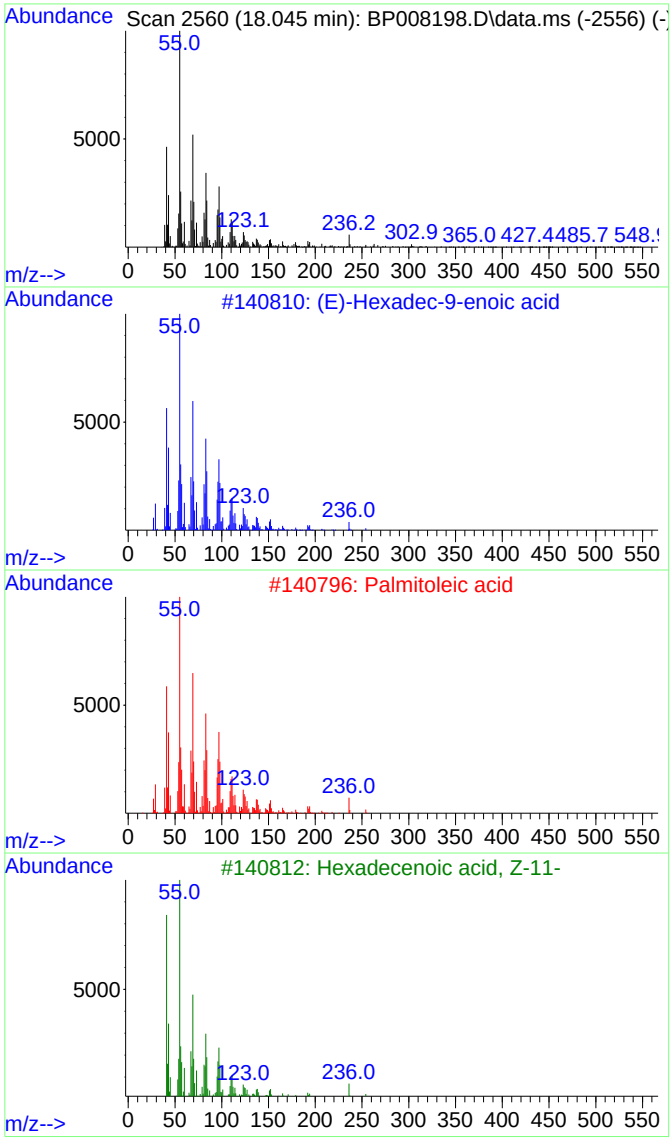
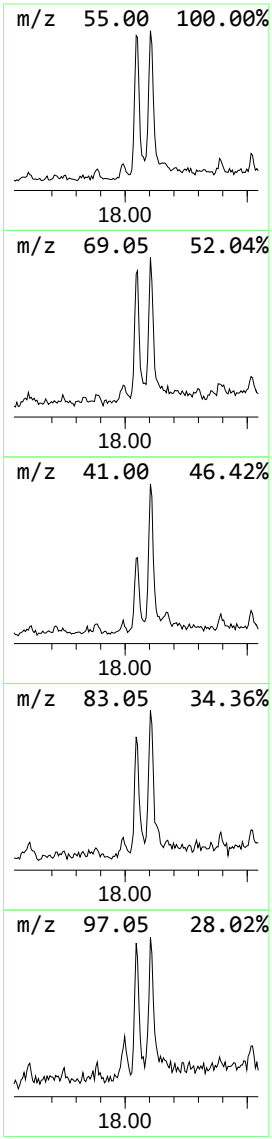
****

Peak Number 3 (E)-Hexadec-9-enoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.045	3.61 ng	202476	Phenanthrene-d10	17.204

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-Hexadec-9-enoic acid	254	C16H30O2	010030-73-6	99
2	Palmitoleic acid	254	C16H30O2	000373-49-9	99
3	Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	99
4	cis-7-Hexadecenoic acid	254	C16H30O2	002416-19-5	99
5	cis-Vaccenic acid	282	C18H34O2	000506-17-2	91





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Instrument :
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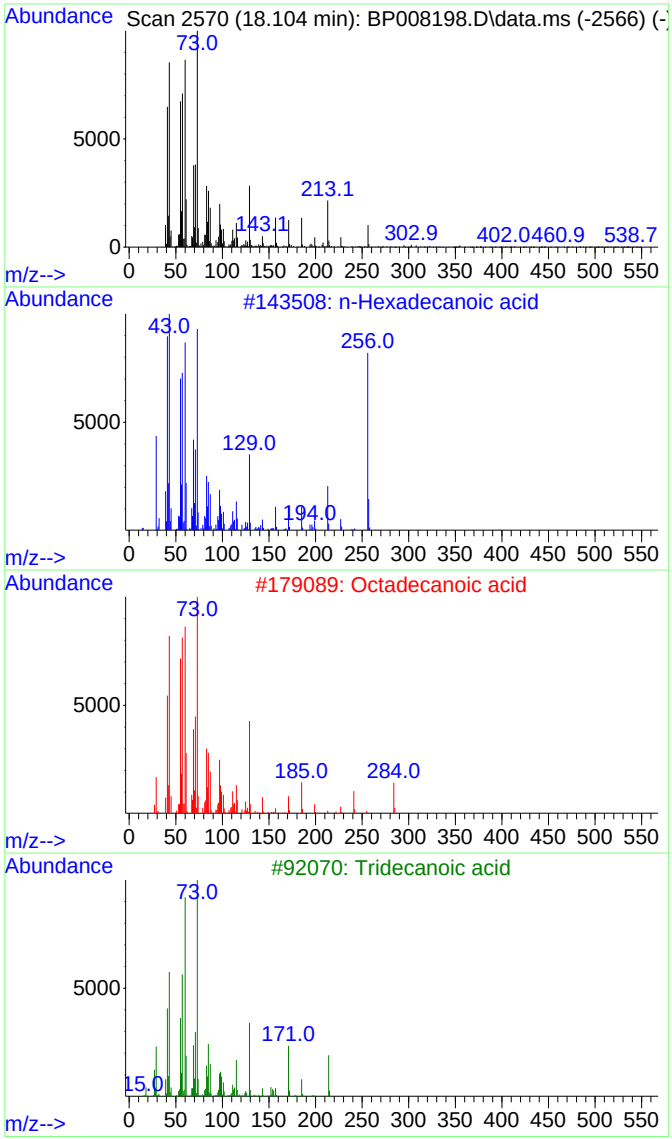
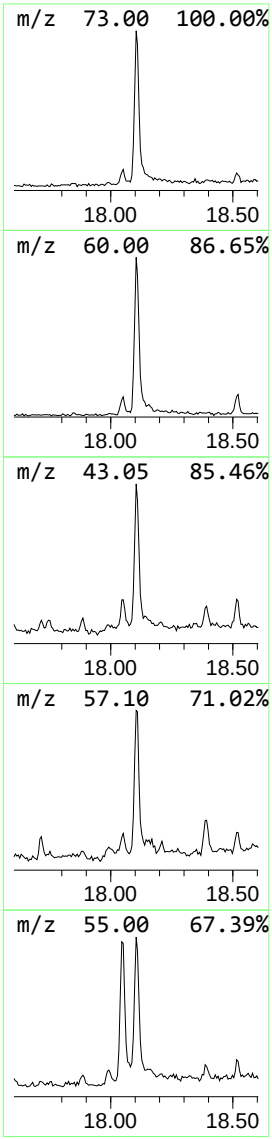
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.104	6.90 ng	387018	Phenanthrene-d10	17.204

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Octadecanoic acid	284	C18H36O2	000057-11-4	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	86
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5	Undecanoic acid	186	C11H22O2	000112-37-8	59





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ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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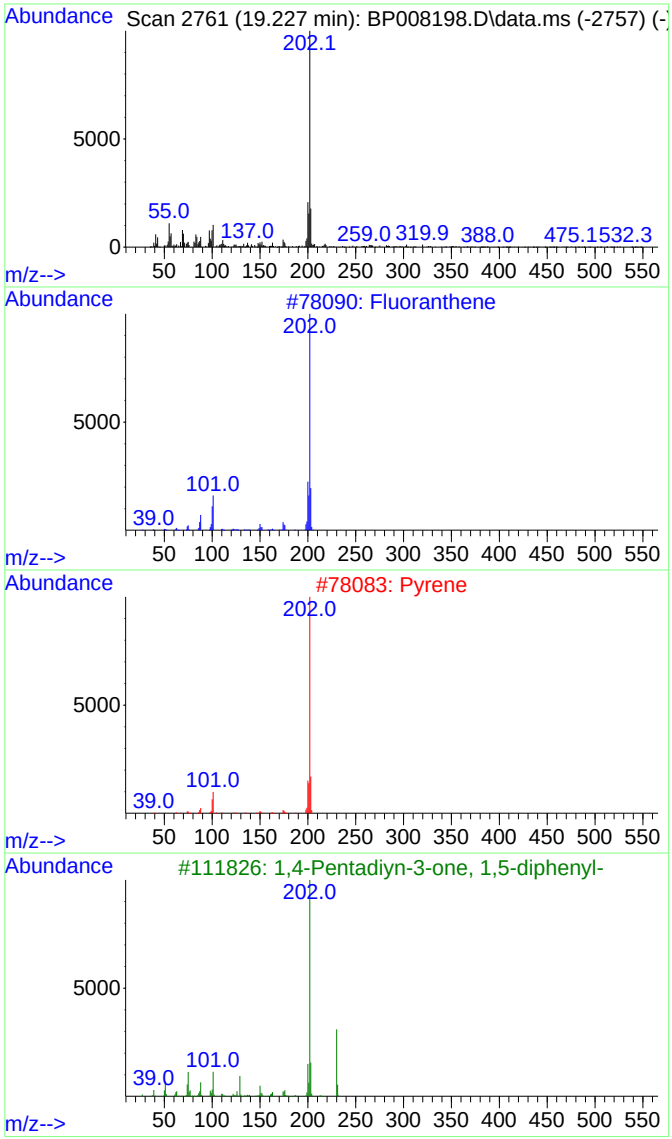
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

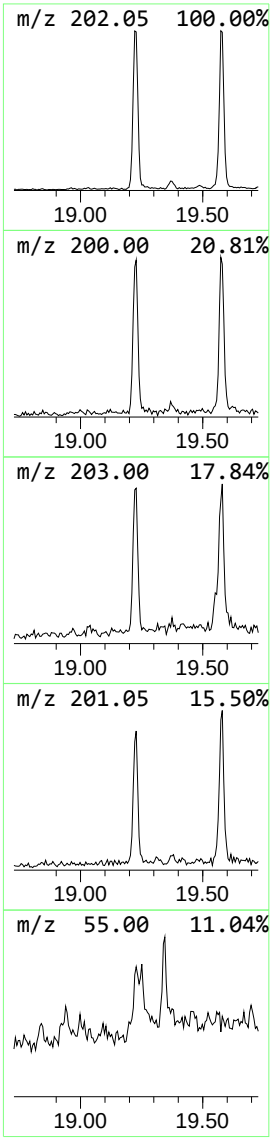
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1,4-Pentadiyn-3-one, 1,5-di... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.227	2.55 ng	143149	Phenanthrene-d10	17.204

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fluoranthene	202	C16H10	000206-44-0	95
2	Pyrene	202	C16H10	000129-00-0	94
3	1,4-Pentadiyn-3-one, 1,5-diphenyl-	230	C17H10O	015814-30-9	72
4	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	68
5	l-Leucine, N-methyl-N-(2-methoxy...	443	C25H49NO5	1000328-54-8	38





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
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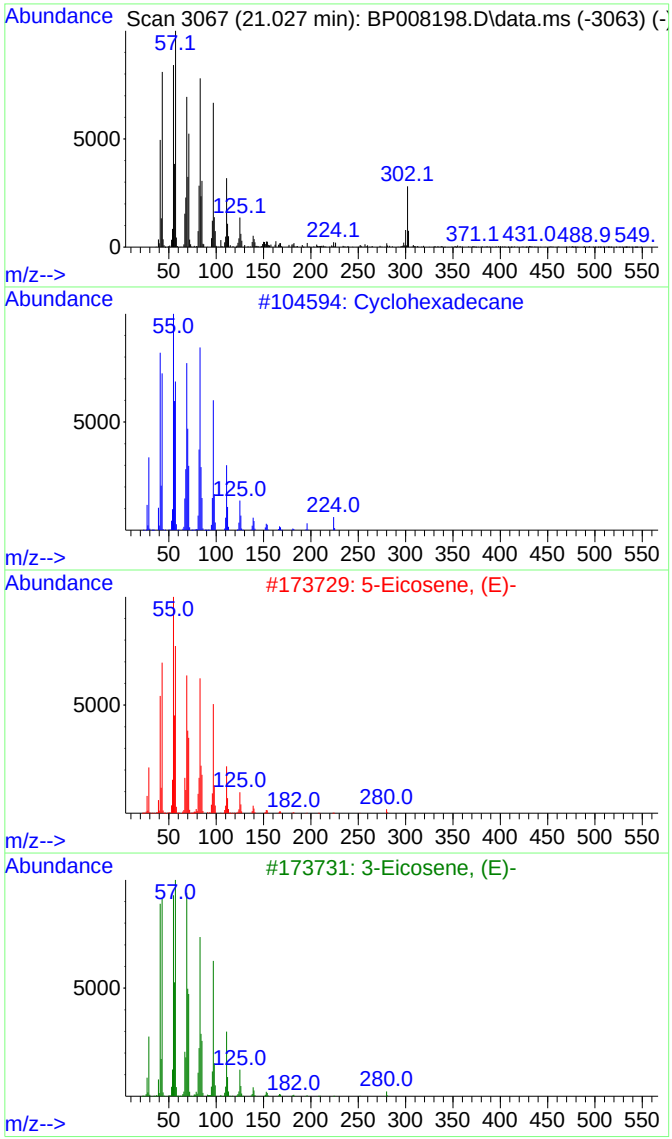
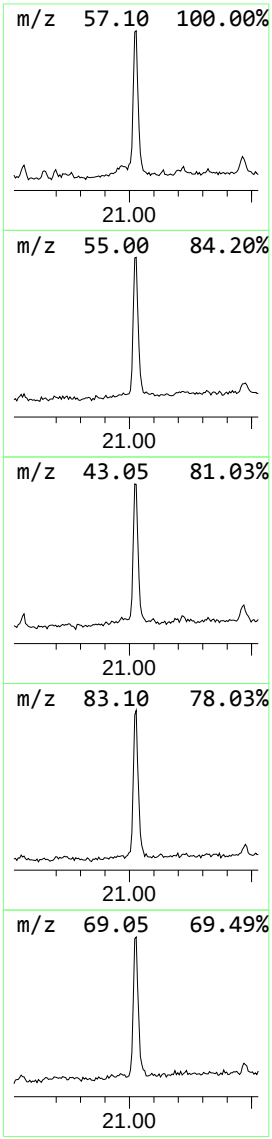
****

Peak Number 6 Cyclohexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.027	10.06 ng	668823	Chrysene-d12	21.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	99
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	96
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	96
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	93
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93





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ALS Vial : 15 Sample Multiplier: 1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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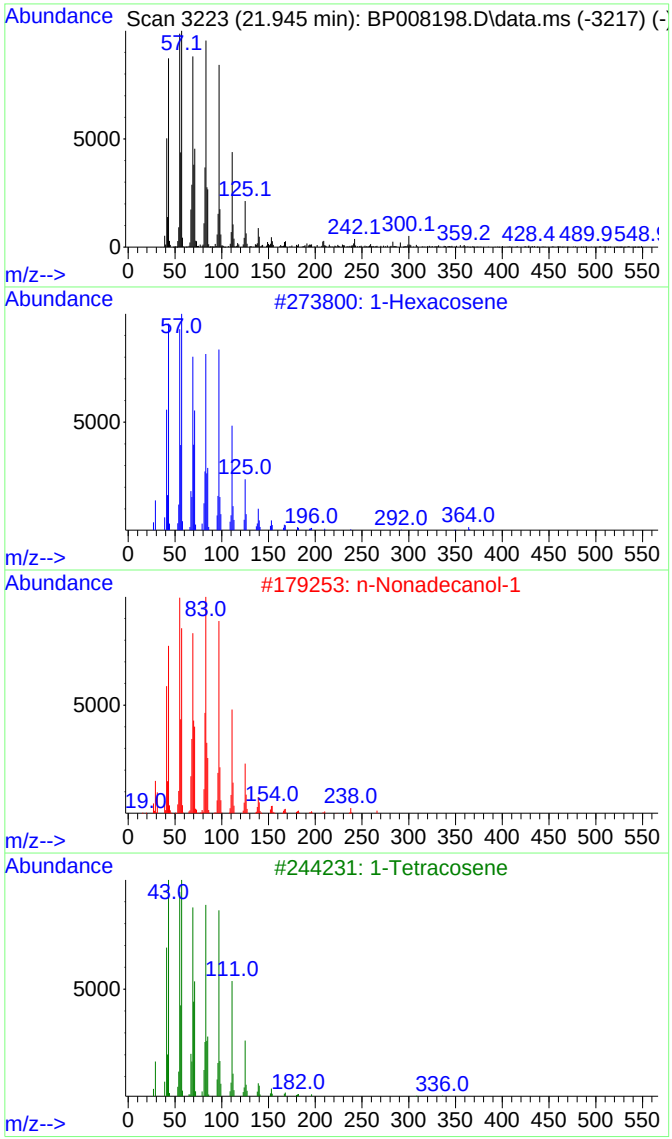
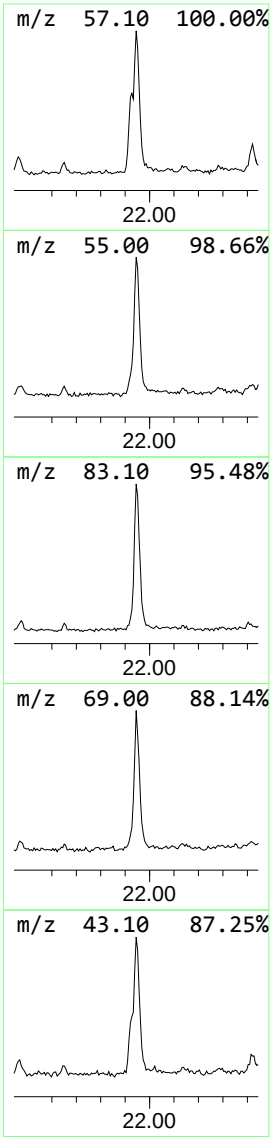
****

Peak Number 7 1-Hexacosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.945	12.66 ng	841345	Chrysene-d12	21.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene	364	C26H52	018835-33-1	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
3	1-Tetracosene	336	C24H48	010192-32-2	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	94
5	9-Tricosene, (Z)-	322	C23H46	027519-02-4	94





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TIC Library : C:\Database\NIST20.L
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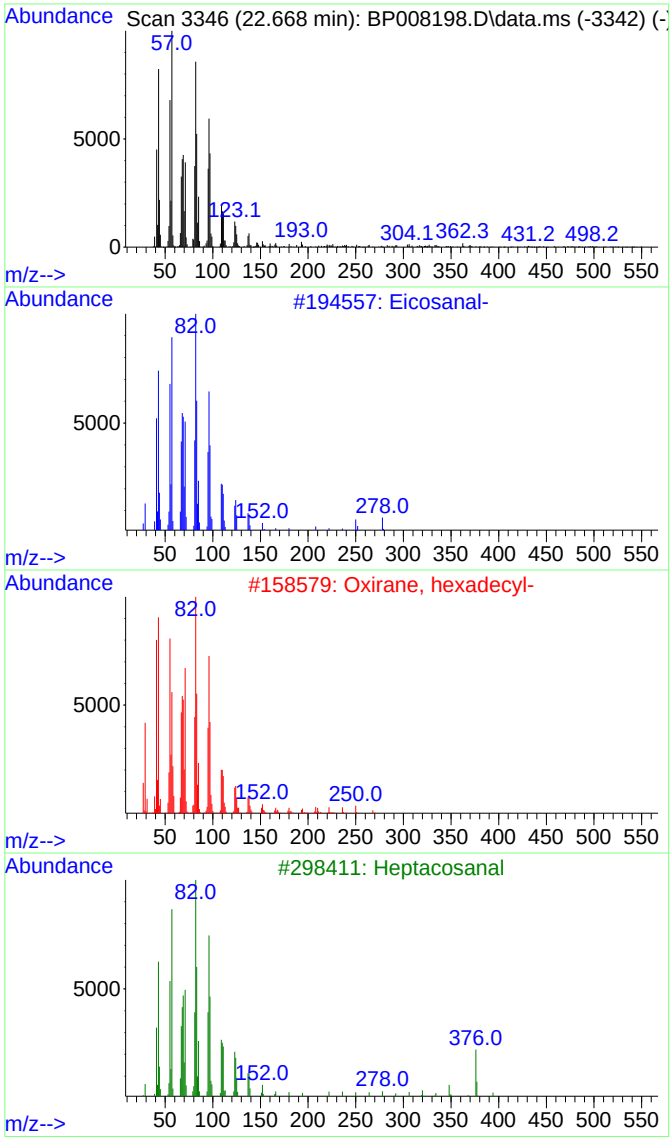
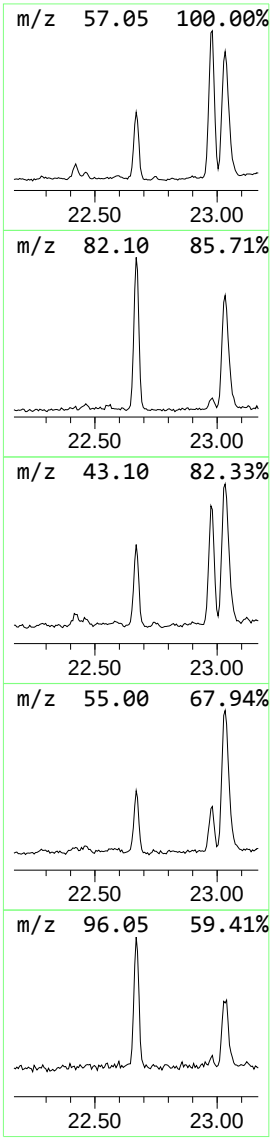
****

Peak Number 8 Eicosanal- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.668	9.53 ng	626577	Perylene-d12	23.704

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosanal-	296	C20H40O	002400-66-0	93
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
3	Heptacosanal	394	C27H54O	072934-03-3	91
4	Octadecanal	268	C18H36O	000638-66-4	90
5	Octacosanal	408	C28H56O	022725-64-0	87





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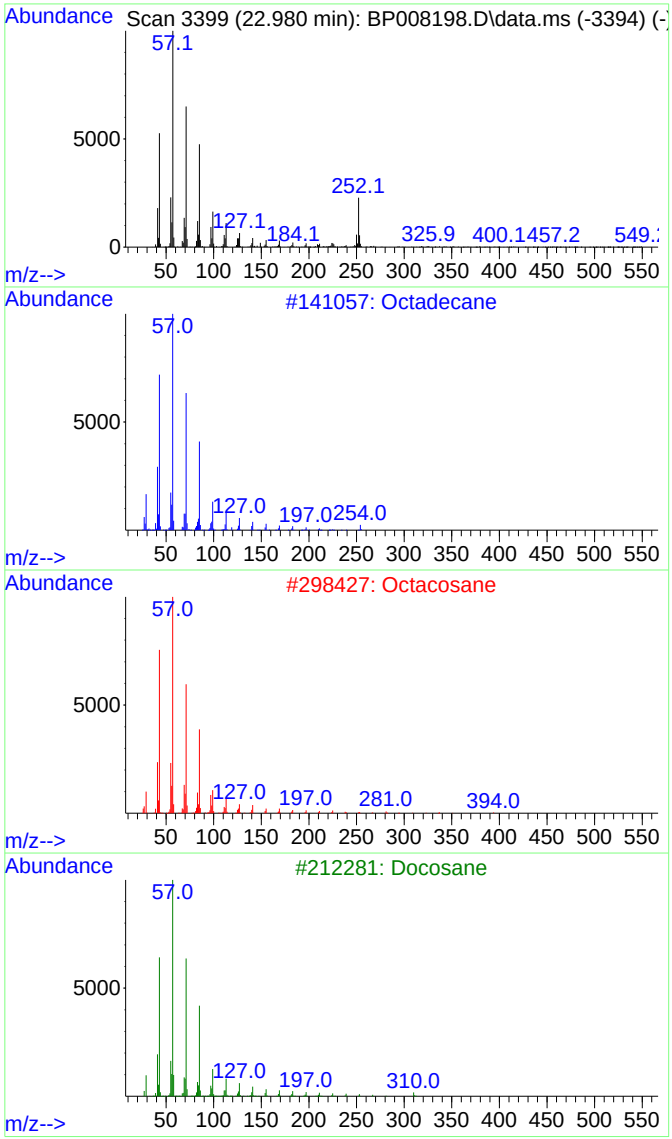
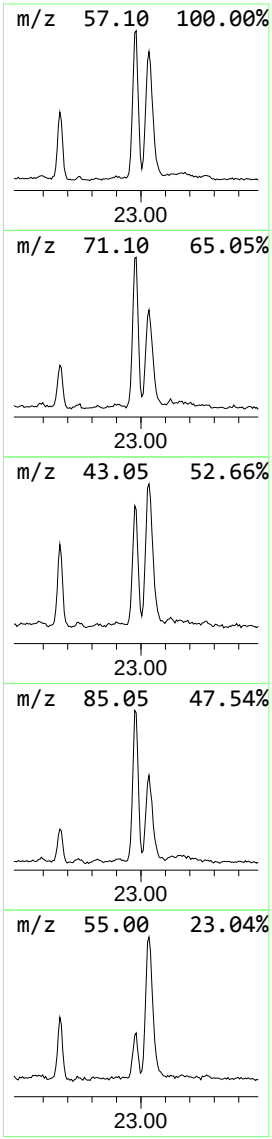
****

Peak Number 9 Octadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.980	10.40 ng	683798	Perylene-d12	23.704

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	95
2	Octacosane	394	C28H58	000630-02-4	95
3	Docosane	310	C22H46	000629-97-0	93
4	Hexacosane	366	C26H54	000630-01-3	90
5	Nonacosane	408	C29H60	000630-03-5	90





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Acq On : 02 Dec 2021 18:52
Operator : CG/JU
Sample : M4877-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PL-2-120121

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.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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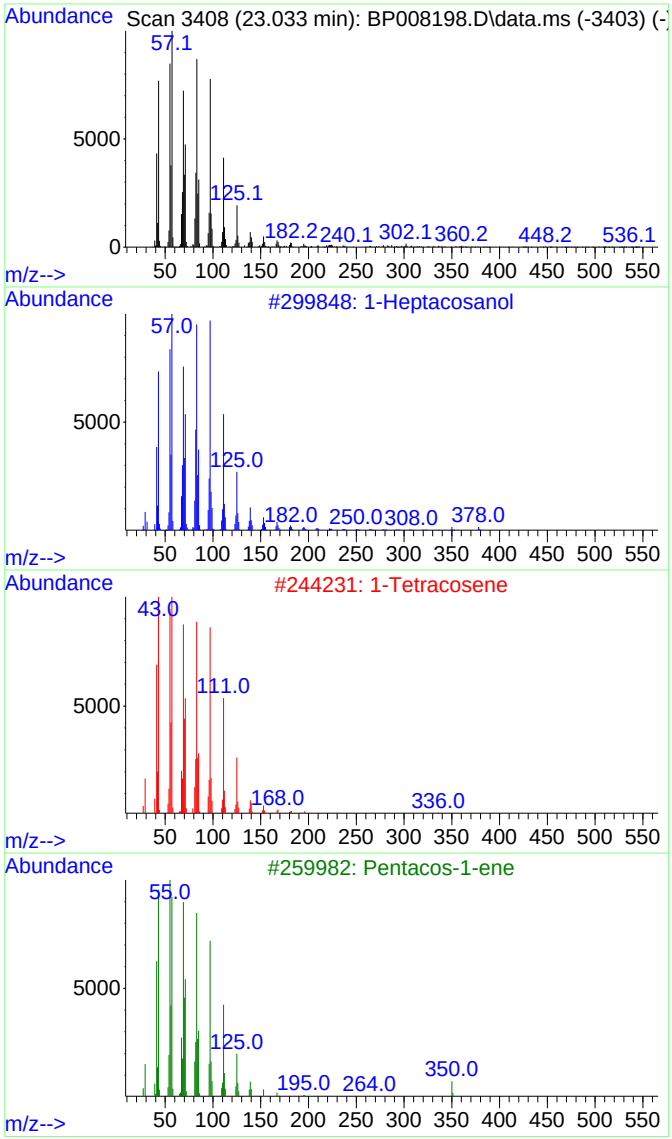
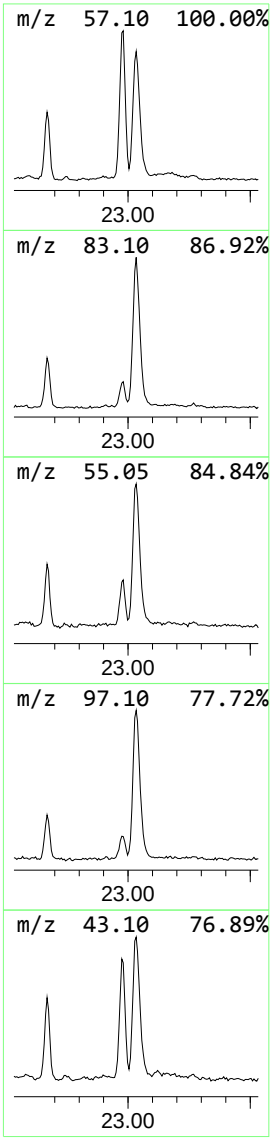
Peak Number 10 1-Heptacosanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.033	21.09 ng	1386340	Perylene-d12	23.704

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	95
2	1-Tetracosene	336	C24H48	010192-32-2	94
3	Pentacos-1-ene	350	C25H50	016980-85-1	94
4	Heptacos-1-ene	378	C27H54	015306-27-1	94
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120221\
Data File : BP008198.D
Acq On : 02 Dec 2021 18:52
Operator : CG/JU
Sample : M4877-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PL-2-120121

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.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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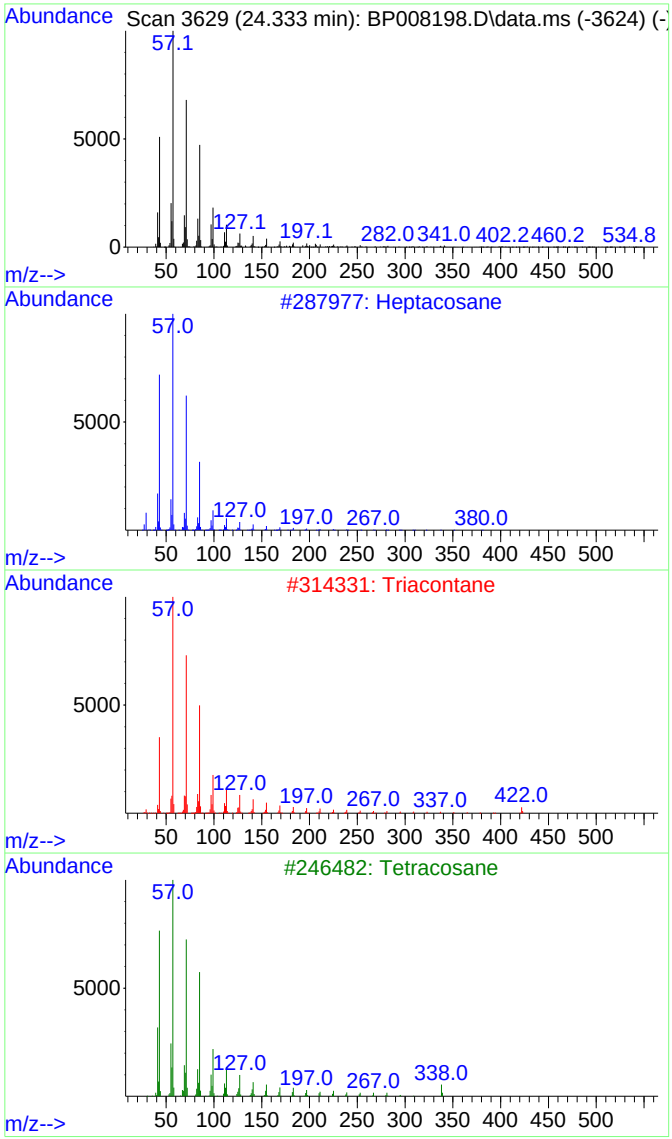
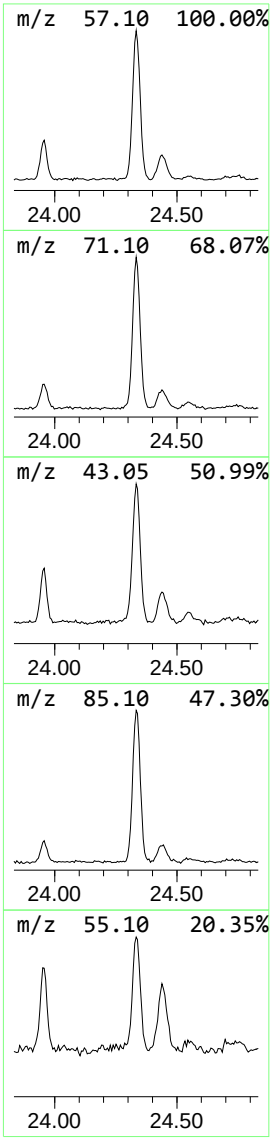
Peak Number 11 Heptacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.333	14.63 ng	961588	Perylene-d12	23.704

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	97
2	Triacontane	422	C30H62	000638-68-6	96
3	Tetracosane	338	C24H50	000646-31-1	95
4	2-Methyltetracosane	352	C25H52	001560-78-7	95
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120221\
Data File : BP008198.D
Acq On : 02 Dec 2021 18:52
Operator : CG/JU
Sample : M4877-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PL-2-120121

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.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
Propane, 1,1-di...	3.046	2.1	ng	55641	1	7.793	522823	20.0
2-Pentanone, 4-...	4.922	11.7	ng	306166	1	7.793	522823	20.0
(E)-Hexadec-9-e...	18.045	3.6	ng	202476	4	17.204	1121270	20.0
n-Hexadecanoic ...	18.104	6.9	ng	387018	4	17.204	1121270	20.0
1,4-Pentadiyn-3...	19.227	2.5	ng	143149	4	17.204	1121270	20.0
Cyclohexadecane	21.027	10.1	ng	668823	5	21.310	1329270	20.0
1-Hexacosene	21.945	12.7	ng	841345	5	21.310	1329270	20.0
Eicosanal-	22.668	9.5	ng	626577	6	23.704	1314430	20.0
Octadecane	22.980	10.4	ng	683798	6	23.704	1314430	20.0
1-Heptacosanol	23.033	21.1	ng	1386340	6	23.704	1314430	20.0
Heptacosane	24.333	14.6	ng	961588	6	23.704	1314430	20.0