LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031323\
Data File : BF132763.D
Acq On : 13 Mar 2023 16:44
Operator : CG\JU
Sample : 01869-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : UPS-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-BF022223.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132763.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.593	337	341	348	rBV	108338	120380	1.64%	0.307%
2	5.193	439	443	454	rVB	904831	937891	12.75%	2.394%
3	5.598	508	512	534	rVB	2199261	2166919	29.47%	5.530%
4	5.981	574	577	581	rBV	179970	153314	2.08%	0.391%
5	6.593	678	681	695	rVB	1339665	1337558	18.19%	3.414%
6	6.969	741	745	749	rBV	1598339	1262544	17.17%	3.222%
7	7.534	837	841	844	rBV	3380765	3459727	47.05%	8.830%
8	7.634	849	858	866	rBV	218367	307124	4.18%	0.784%
9	8.251	960	963	967	rBV	2043968	1644674	22.37%	4.197%
10	9.328	1142	1146	1149	rBV	6747809	6031496	82.02%	15.393%
11	10.010	1259	1262	1266	rVB	2326399	1992588	27.10%	5.085%
12	10.728	1380	1384	1387	rVB	1477184	1243947	16.92%	3.175%
13	10.810	1393	1398	1401	rBV	4762459	4425023	60.17%	11.293%
14	11.033	1433	1436	1442	rVB	151834	122889	1.67%	0.314%
15	11.504	1512	1516	1520	rBV	2465208	2193564	29.83%	5.598%
16	12.016	1599	1603	1608	rBV	752496	790808	10.75%	2.018%
17	12.804	1734	1737	1749	rBV	353646	416637	5.67%	1.063%
18	13.098	1782	1787	1790	rBV	7133595	7353700	100.00%	18.768%
19	13.974	1933	1936	1946	rBV	213189	327312	4.45%	0.835%
20	14.157	1963	1967	1971	rBV	1424512	1367941	18.60%	3.491%
21	14.245	1978	1982	1988	rBV	144676	145204	1.97%	0.371%
22	15.004	2107	2111	2115	rVB	177990	175597	2.39%	0.448%
23	15.692	2223	2228	2235	rVB2	951894	1205930	16.40%	3.078%

Sum of corrected areas: 39182767

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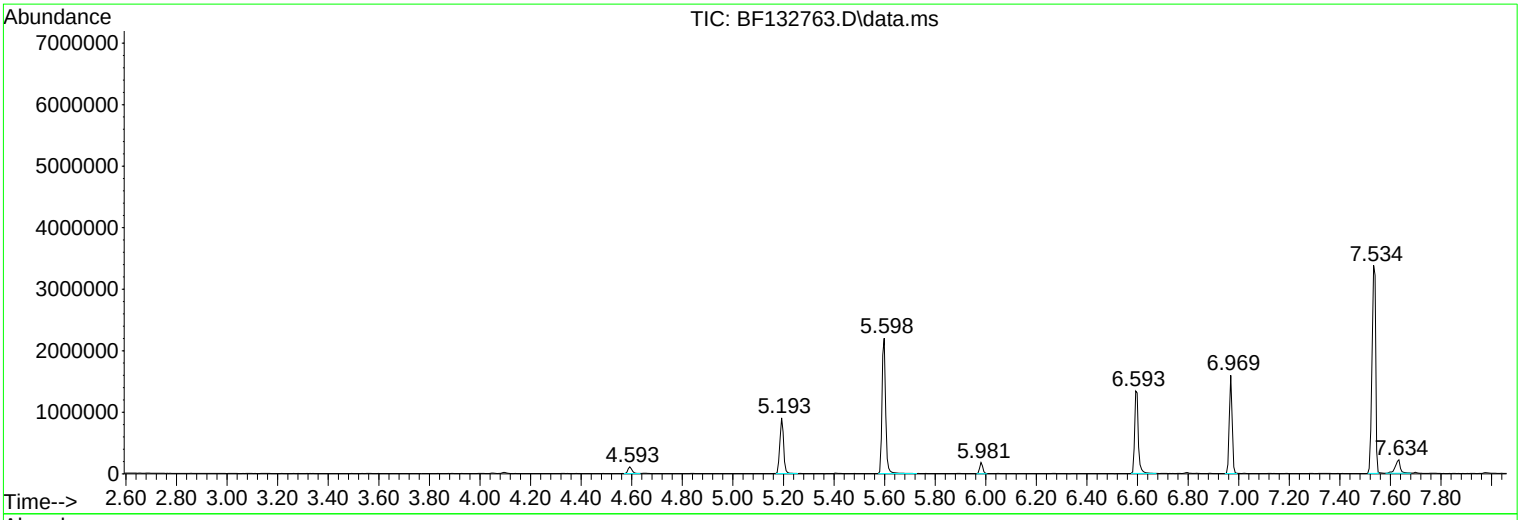
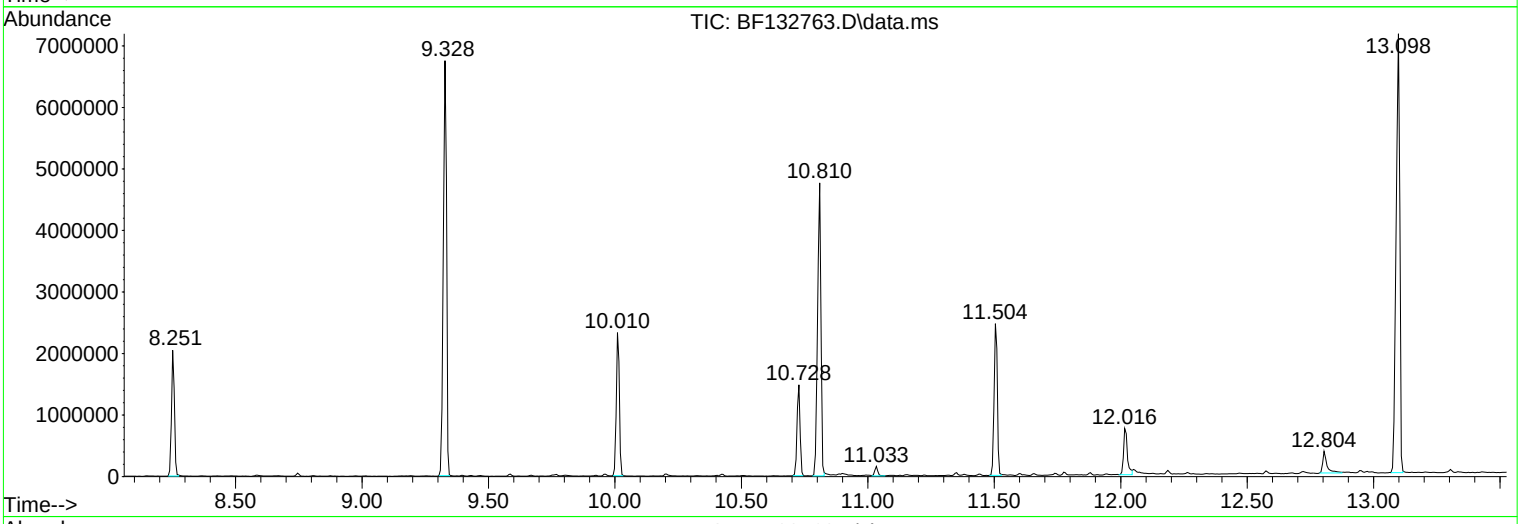
Misc :
ALS Vial : 11 Sample Multiplier: 1

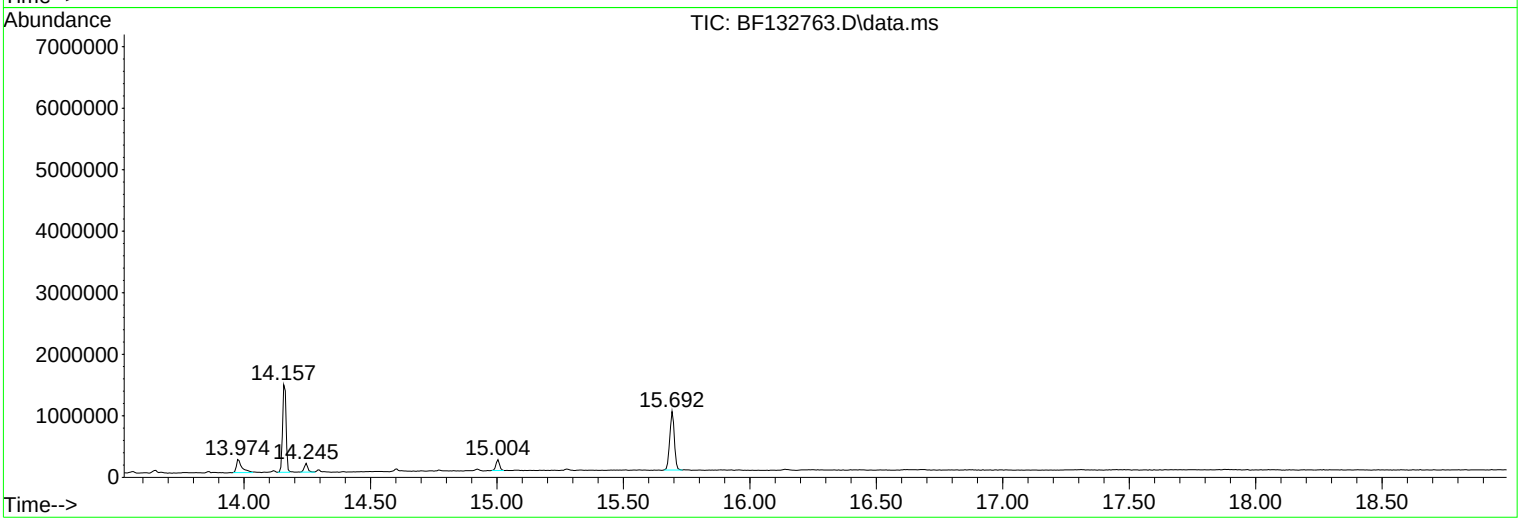
Instrument :
BNA_F
ClientSampleId :
UPS-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.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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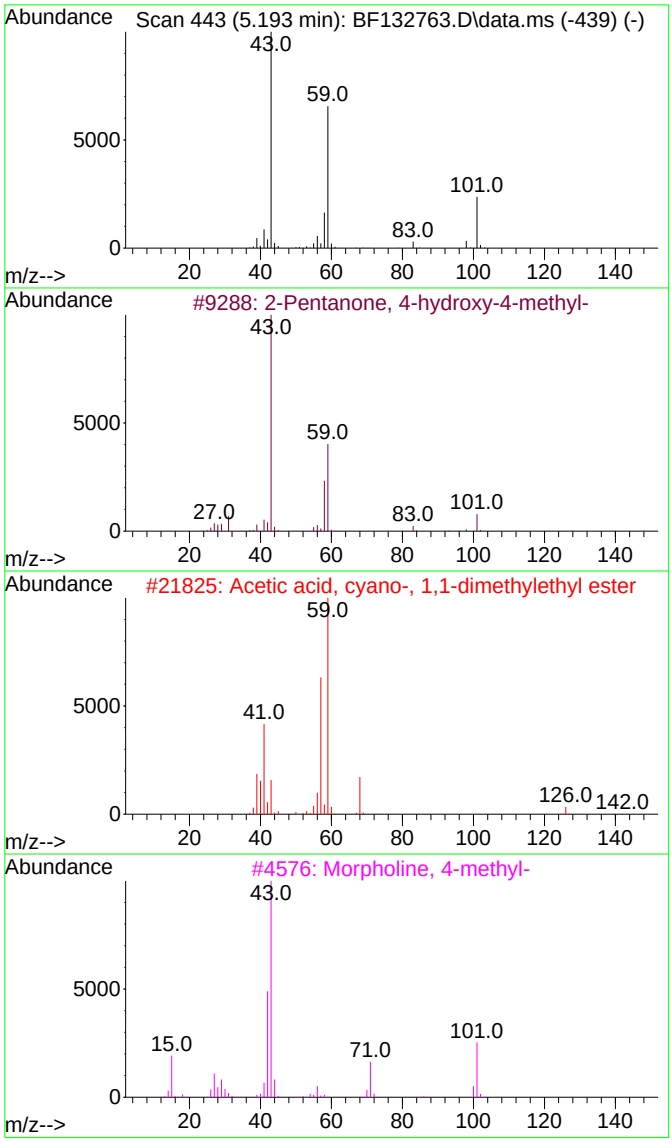
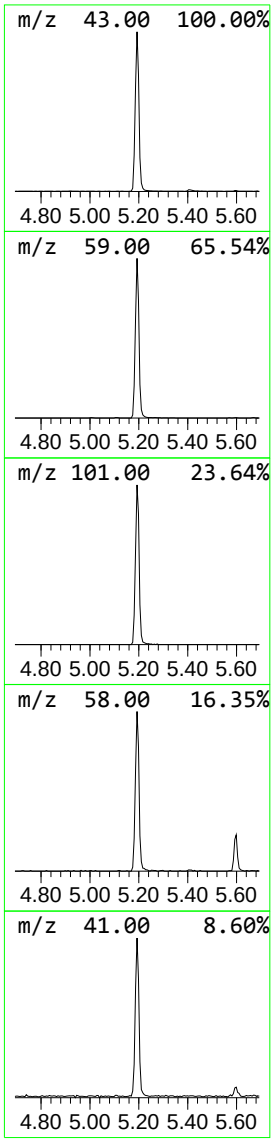
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.193	14.86 ng	937891	1,4-Dichlorobenzene-d4	6.969

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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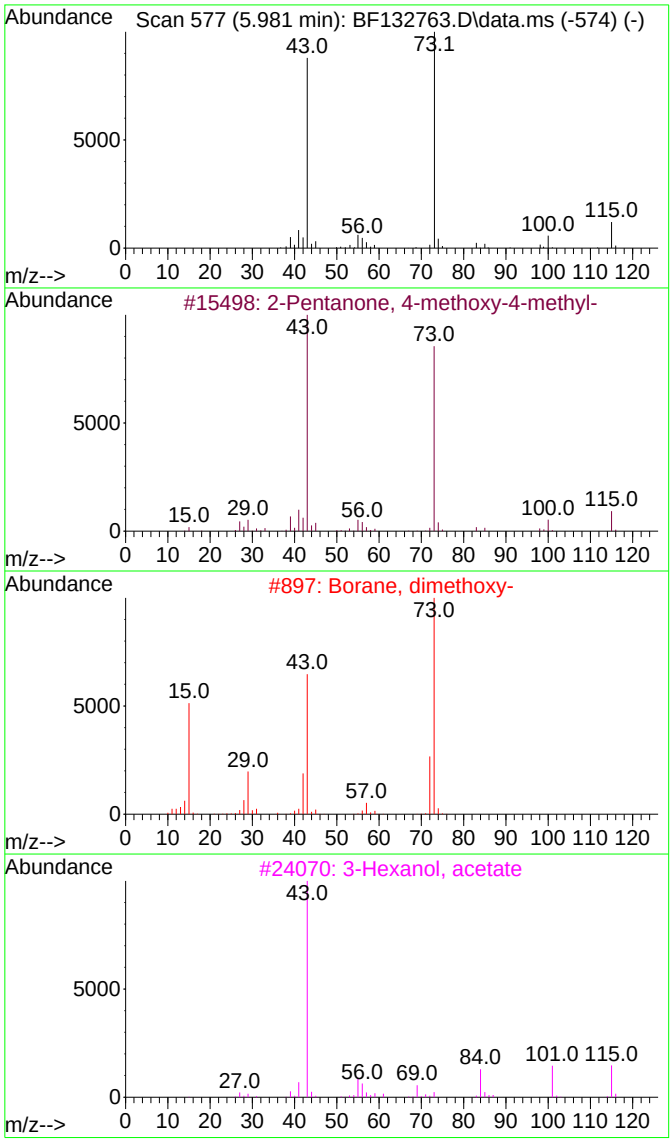
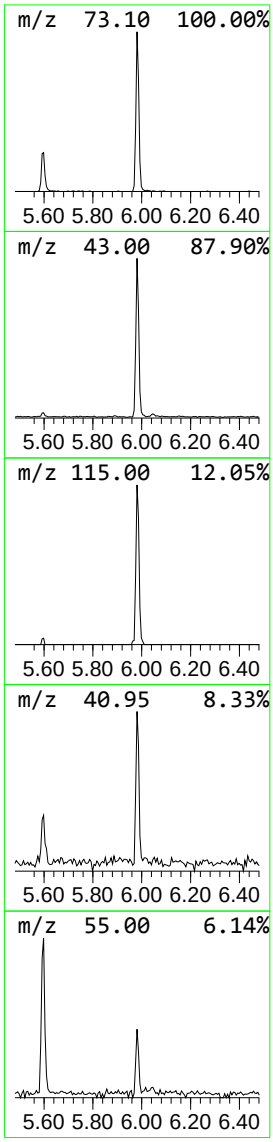
****
Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.981	2.43 ng	153314	1,4-Dichlorobenzene-d4	6.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	38
3	3-Hexanol, acetate	144	C8H16O2	040780-64-1	37
4	Butane, 2-methoxy-2,3,3-trimethyl-	130	C8H18O	027705-21-1	23
5	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	17





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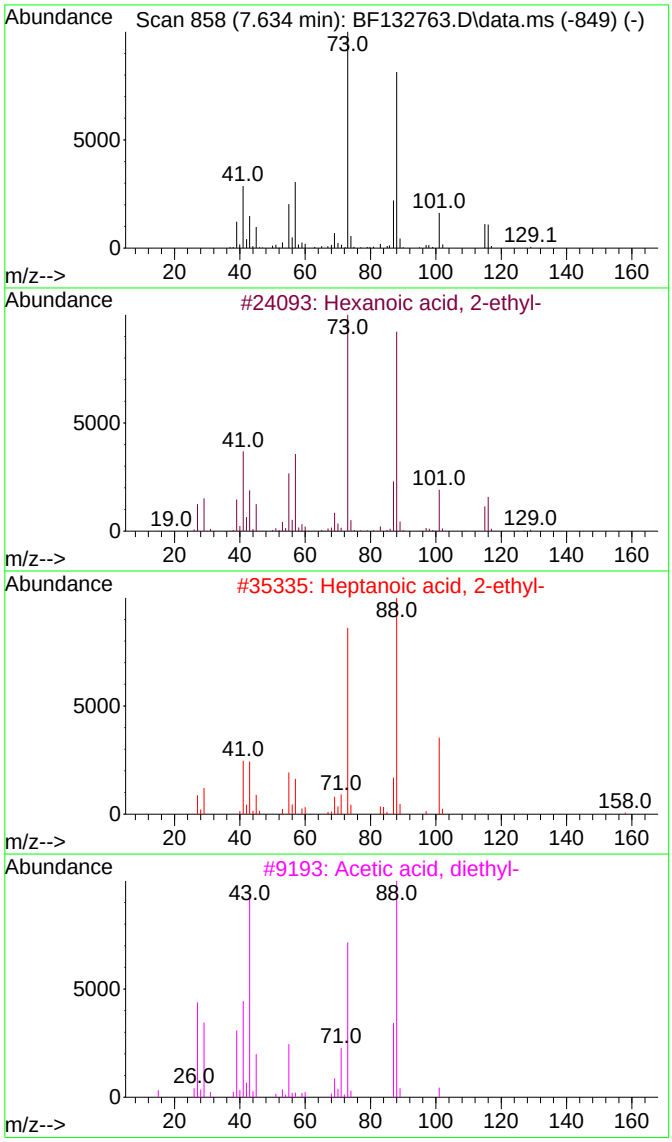
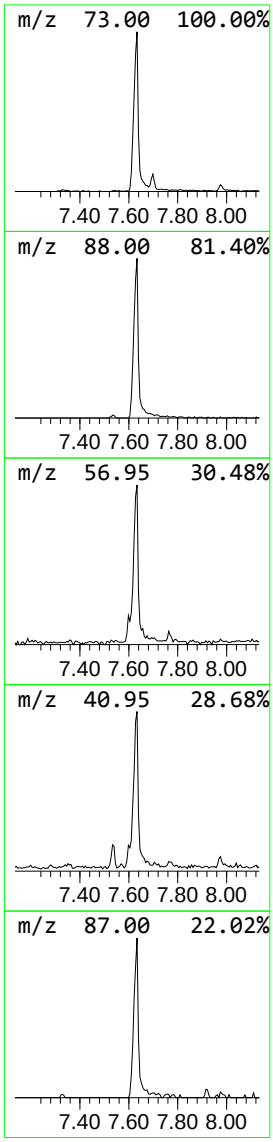
****

Peak Number 3 Hexanoic acid, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.634	3.73 ng	307124	Naphthalene-d8	8.251

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	59
3	Acetic acid, diethyl-	116	C6H12O2	000088-09-5	59
4	2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	45
5	Methyl-4-deoxy-2,3-di-O-methyl.b...	218	C9H14O6	1000312-09-9	42





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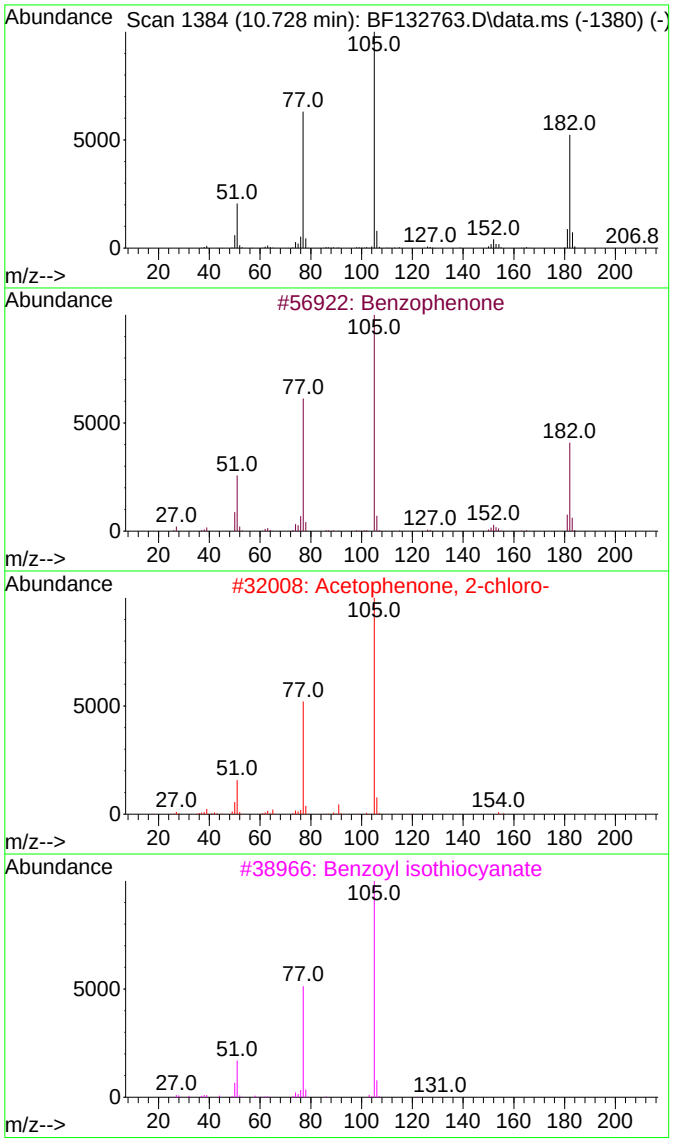
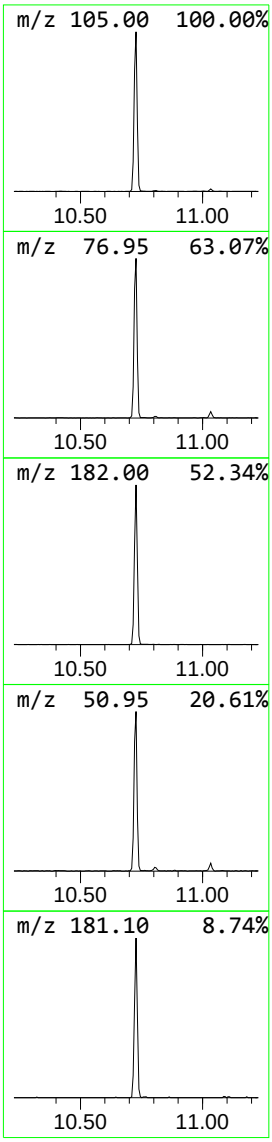
****

Peak Number 4 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.727	12.49 ng	1243950	Acenaphthene-d10	10.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3	Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47
4	Vinyl benzoate	148	C9H8O2	000769-78-8	47
5	Methyl 2-benzoyl-4-cyanobutanoate	231	C13H13NO3	1010486-83-8	47





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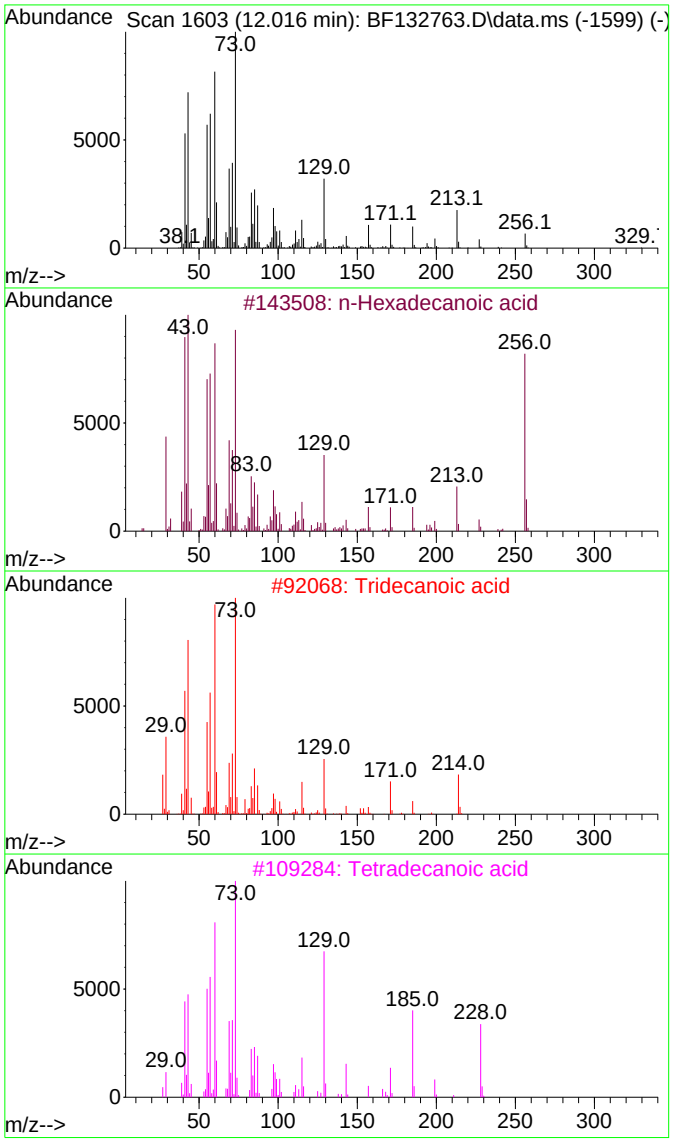
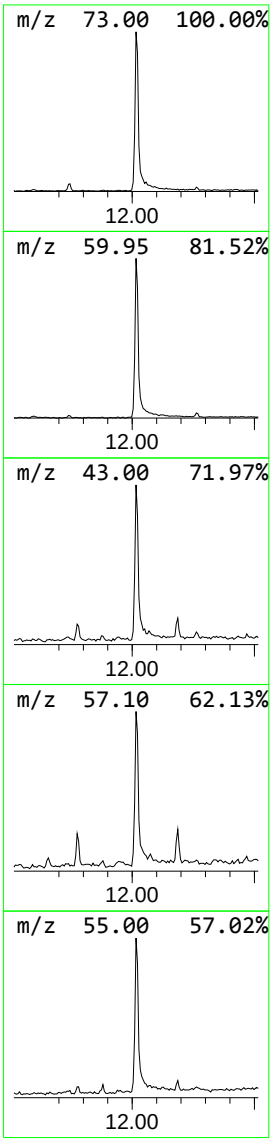
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.016	7.21 ng	790808	Phenanthrene-d10	11.504

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	81
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5	Dodecanoic acid	200	C12H24O2	000143-07-7	68





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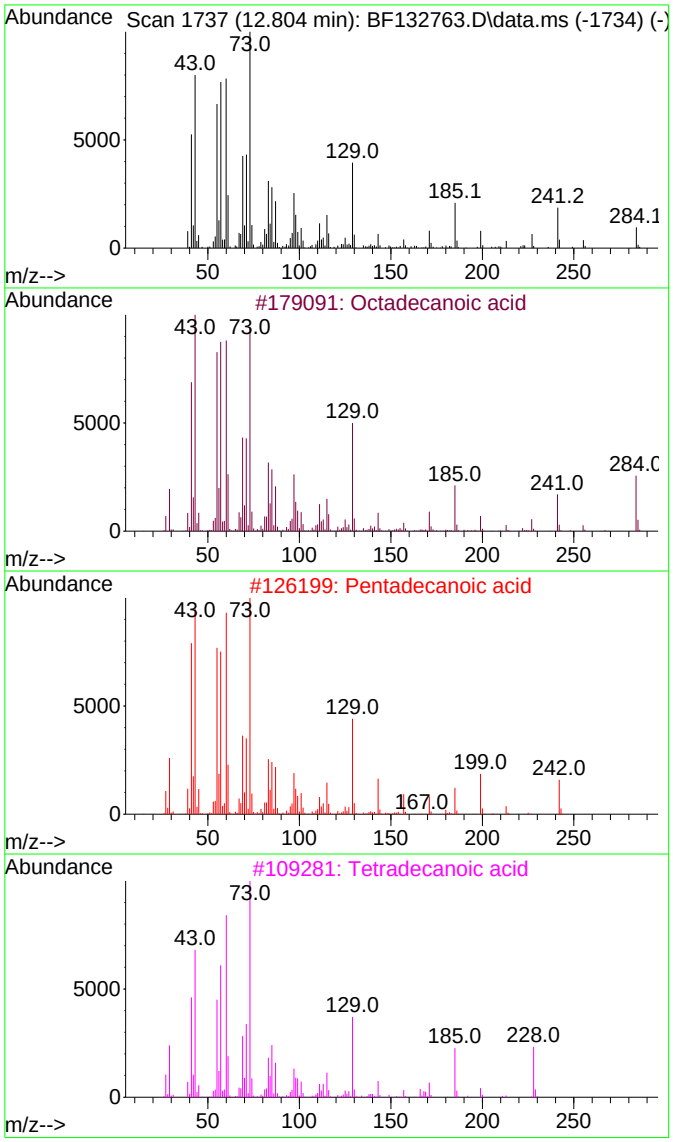
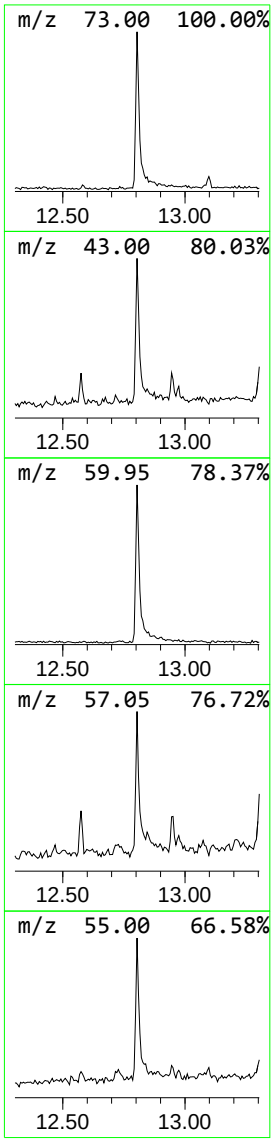
****

Peak Number 6 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.804	3.80 ng	416637	Phenanthrene-d10	11.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	52





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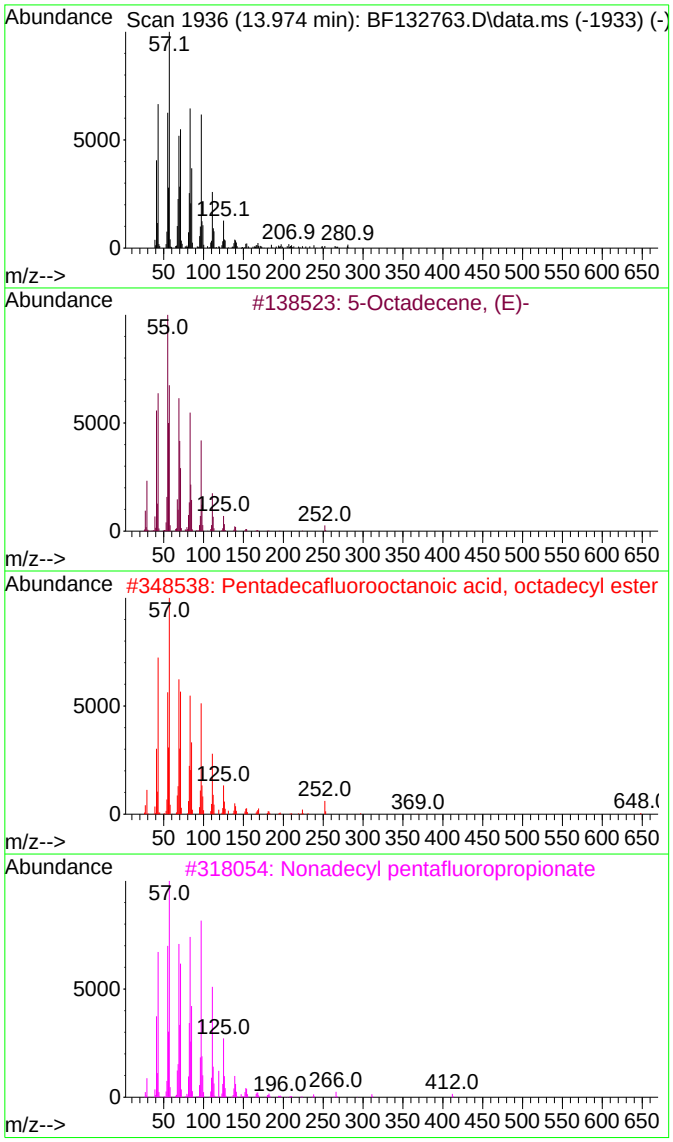
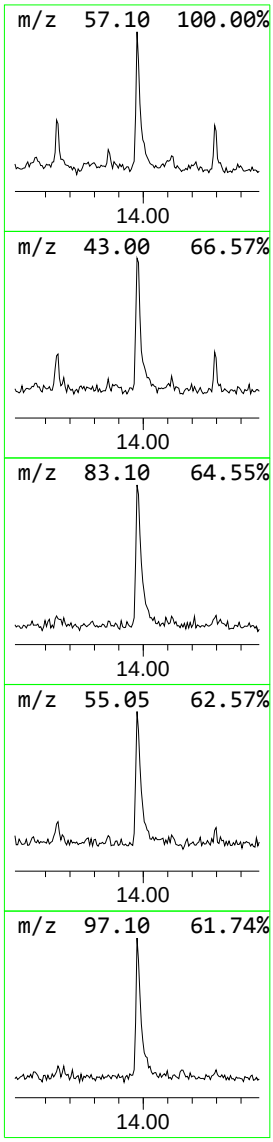
****

Peak Number 7 5-Octadecene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.974	4.79 ng	327312	Chrysene-d12	14.157

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	91
2	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
3	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
4	17-Pentatriacontene	491	C35H70	006971-40-0	91
5	8-Heptadecene	238	C17H34	002579-04-6	89





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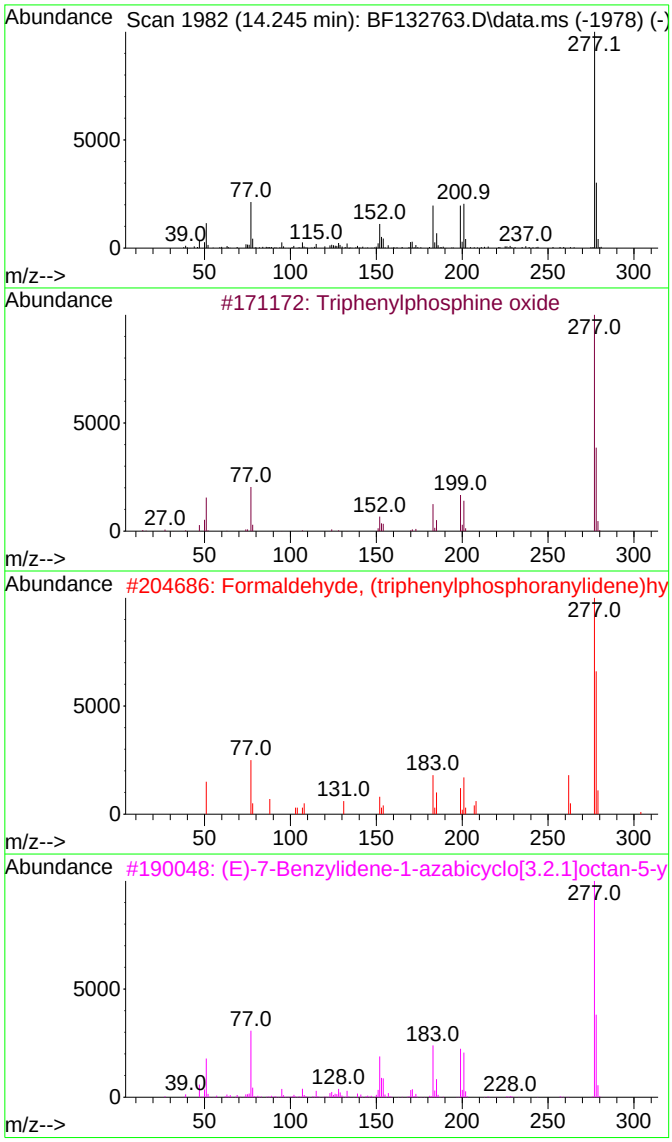
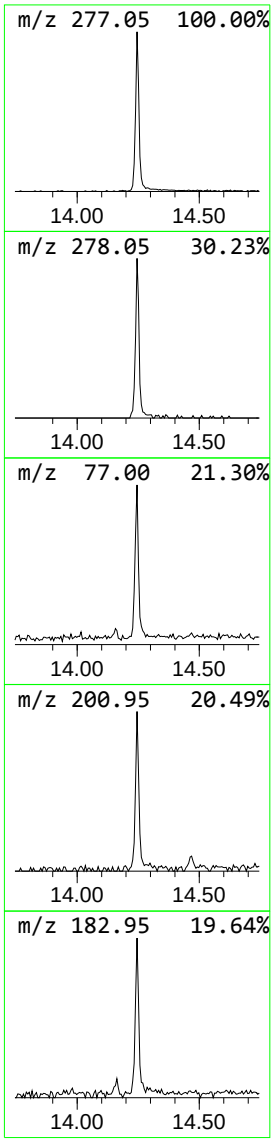
Peak Number 8 Triphenylphosphine oxide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.245	2.12 ng	145204	Chrysene-d12	14.157

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	91
2	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
3	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	49
4	Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	35
5	2-Propenoic acid, 2-cyano-3-(3-p...	277	C18H15NO2	1000080-00-3	25





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BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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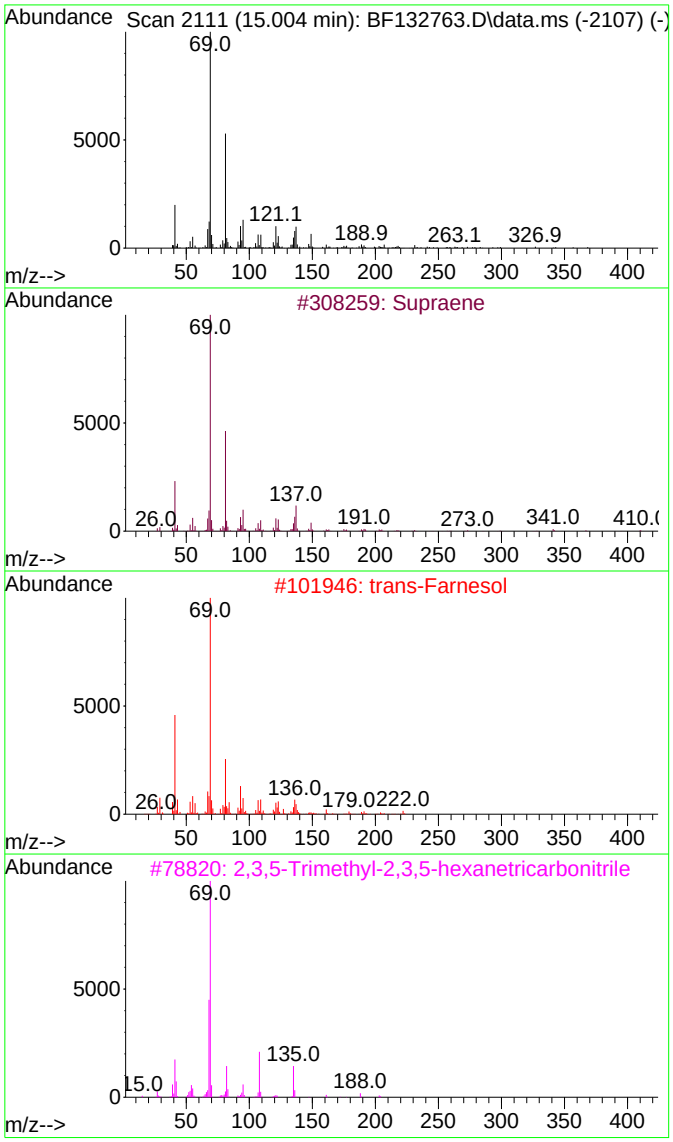
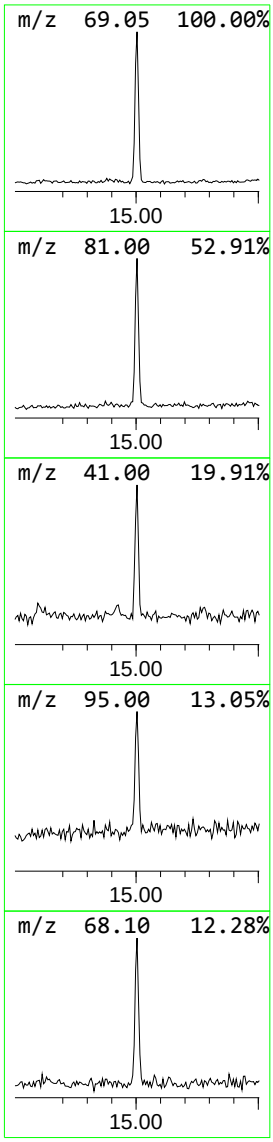
Peak Number 9 Supraene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.004	2.91 ng	175597	Perylene-d12	15.692

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	trans-Farnesol	222	C15H26O	000106-28-5	64
3	2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	50
4	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	50
5	2-Butenoic acid, 4-nitrophenyl e...	207	C10H9NO4	035665-90-8	49





Tentatively Identified Compound (LSC) summary

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Sample : 01869-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UPS-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.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-...	5.193	14.9	ng	937891	1	6.969	1262540	20.0
2-Pentanone, 4-...	5.981	2.4	ng	153314	1	6.969	1262540	20.0
Hexanoic acid, ...	7.634	3.7	ng	307124	2	8.251	1644670	20.0
Benzophenone	10.727	12.5	ng	1243950	3	10.010	1992590	20.0
n-Hexadecanoic ...	12.016	7.2	ng	790808	4	11.504	2193560	20.0
Octadecanoic acid	12.804	3.8	ng	416637	4	11.504	2193560	20.0
5-Octadecene, (E)-	13.974	4.8	ng	327312	5	14.157	1367940	20.0
Triphenylphosph...	14.245	2.1	ng	145204	5	14.157	1367940	20.0
Supraene	15.004	2.9	ng	175597	6	15.692	1205930	20.0