LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030823\
Data File : BF132701.D
Acq On : 08 Mar 2023 21:04
Operator : CG\JU
Sample : 01829-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-08-20230306

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: BF132701.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.222	443	448	461	rVB	1217320	1479173	44.34%	5.002%
2	5.616	511	515	518	rBV	3116137	2915902	87.41%	9.861%
3	5.834	549	552	556	rBV2	48520	46287	1.39%	0.157%
4	6.616	680	685	688	rBV	2901777	2849640	85.42%	9.637%
5	6.987	744	748	752	rBV	1150052	907457	27.20%	3.069%
6	7.039	753	757	763	rBV	89919	77533	2.32%	0.262%
7	7.392	813	817	819	rBV	50391	42330	1.27%	0.143%
8	7.551	840	844	847	rBV	2245392	1886731	56.56%	6.381%
9	8.269	963	966	970	rBV	1336597	1152693	34.55%	3.898%
10	9.345	1145	1149	1152	rBV	4089793	3335972	100.00%	11.282%
11	10.033	1262	1266	1269	rBV	1425426	1197796	35.91%	4.051%
12	10.745	1383	1387	1390	rBV	295476	242971	7.28%	0.822%
13	10.822	1396	1400	1404	rBV	1893089	1778649	53.32%	6.015%
14	11.122	1447	1451	1453	rBV	175743	140644	4.22%	0.476%
15	11.292	1477	1480	1486	rVB	105223	92590	2.78%	0.313%
16	11.527	1516	1520	1523	rBV	1301335	1090606	32.69%	3.688%
17	11.622	1533	1536	1542	rVB4	51708	49604	1.49%	0.168%
18	12.039	1603	1607	1611	rBV	396439	375984	11.27%	1.272%
19	12.074	1611	1613	1620	rVB	35090	40889	1.23%	0.138%
20	12.216	1634	1637	1643	rVB2	34602	42245	1.27%	0.143%
21	12.751	1722	1728	1729	rBV2	64479	86109	2.58%	0.291%
22	12.763	1729	1730	1737	rVV2	69898	77560	2.32%	0.262%
23	12.827	1738	1741	1748	rVV	128108	137898	4.13%	0.466%
24	12.921	1754	1757	1761	rVB	81417	69573	2.09%	0.235%
25	12.998	1768	1770	1778	rVB	76645	85383	2.56%	0.289%
26	13.116	1786	1790	1794	rBV	3236324	2825737	84.71%	9.556%
27	13.327	1817	1826	1829	rBV4	33412	68706	2.06%	0.232%
28	13.627	1874	1877	1881	rVB	42862	40680	1.22%	0.138%
29	13.974	1931	1936	1939	rBV	310257	335522	10.06%	1.135%
30	14.004	1939	1941	1953	rVB	346497	474430	14.22%	1.604%
31	14.145	1961	1965	1969	rBV	2339112	2081106	62.38%	7.038%
32	14.186	1969	1972	1975	rVB	1073050	971279	29.12%	3.285%
33	14.286	1986	1989	1991	rBV	69340	70210	2.10%	0.237%
34	14.310	1991	1993	1997	rVV	257432	229584	6.88%	0.776%
35	14.351	1997	2000	2002	rVV	343599	315419	9.46%	1.067%
36	14.380	2002	2005	2007	rVV	132244	127753	3.83%	0.432%

LSC Area Percent Report

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Operator : CG\JU
Sample : 01829-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-08-20230306

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

37	14.398	2007	2008	2011	rVB	110892	86851	2.60%	0.294%
38	14.633	2044	2048	2055	rBV4	63076	113240	3.39%	0.383%
39	14.704	2057	2060	2065	rVV3	52092	71899	2.16%	0.243%
40	14.804	2074	2077	2080	rVB	85747	77185	2.31%	0.261%
41	14.951	2099	2102	2106	rVB3	41667	54589	1.64%	0.185%
42	15.174	2138	2140	2144	rVB2	54782	59760	1.79%	0.202%
43	15.315	2161	2164	2168	rVB	58498	67280	2.02%	0.228%
44	15.592	2209	2211	2219	rVB	45066	56794	1.70%	0.192%
45	15.727	2229	2234	2244	rVB2	763168	1012825	30.36%	3.425%
46	16.192	2309	2313	2319	rVB2	73675	117675	3.53%	0.398%
47	16.262	2321	2325	2334	rVV5	46173	109121	3.27%	0.369%

Sum of corrected areas: 29569864

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Instrument :
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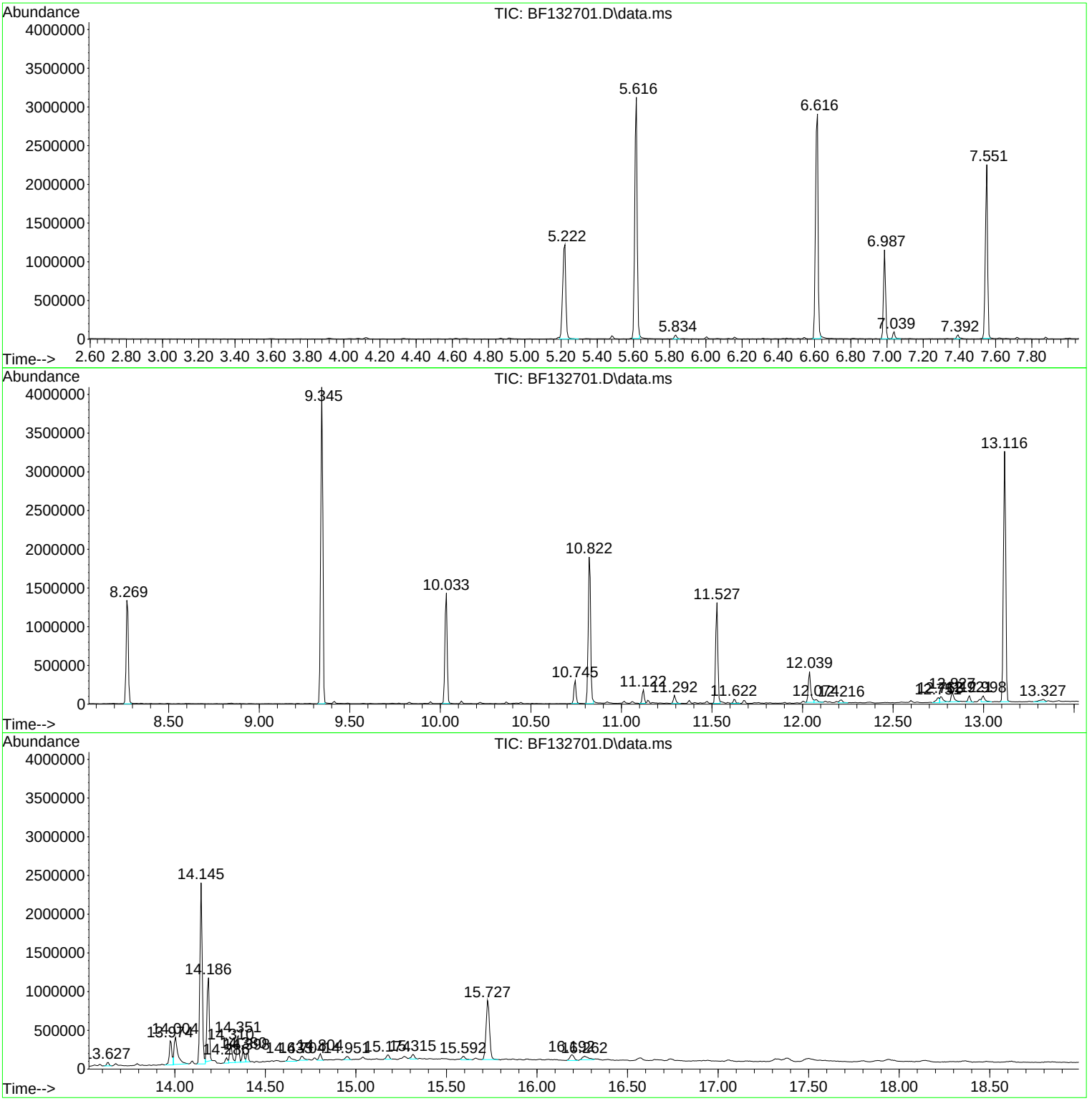
ClientSampleId :
SS-08-20230306

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030823\
Data File : BF132701.D
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Operator : CG\JU
Sample : 01829-08
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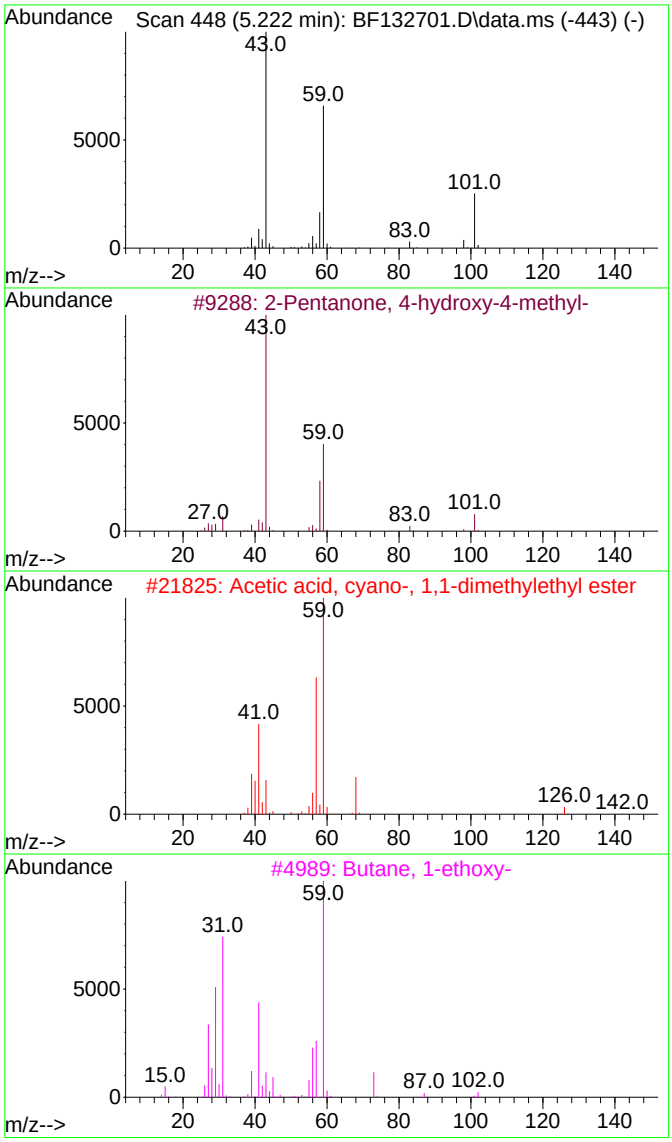
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

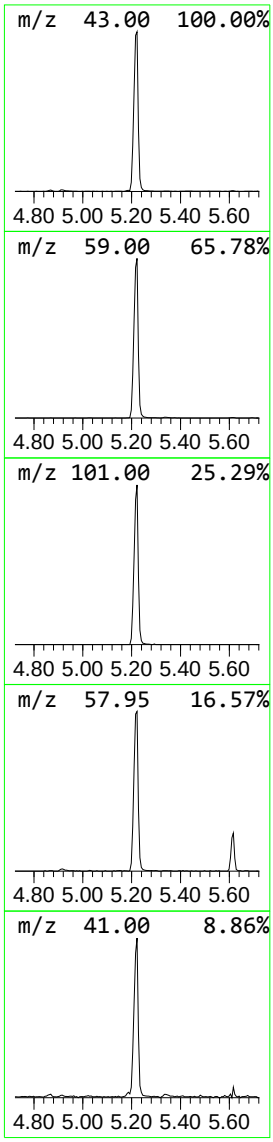
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.222	32.60 ng	1479170	1,4-Dichlorobenzene-d4	6.987

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	17
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





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Acq On : 08 Mar 2023 21:04
Operator : CG\JU
Sample : 01829-08
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

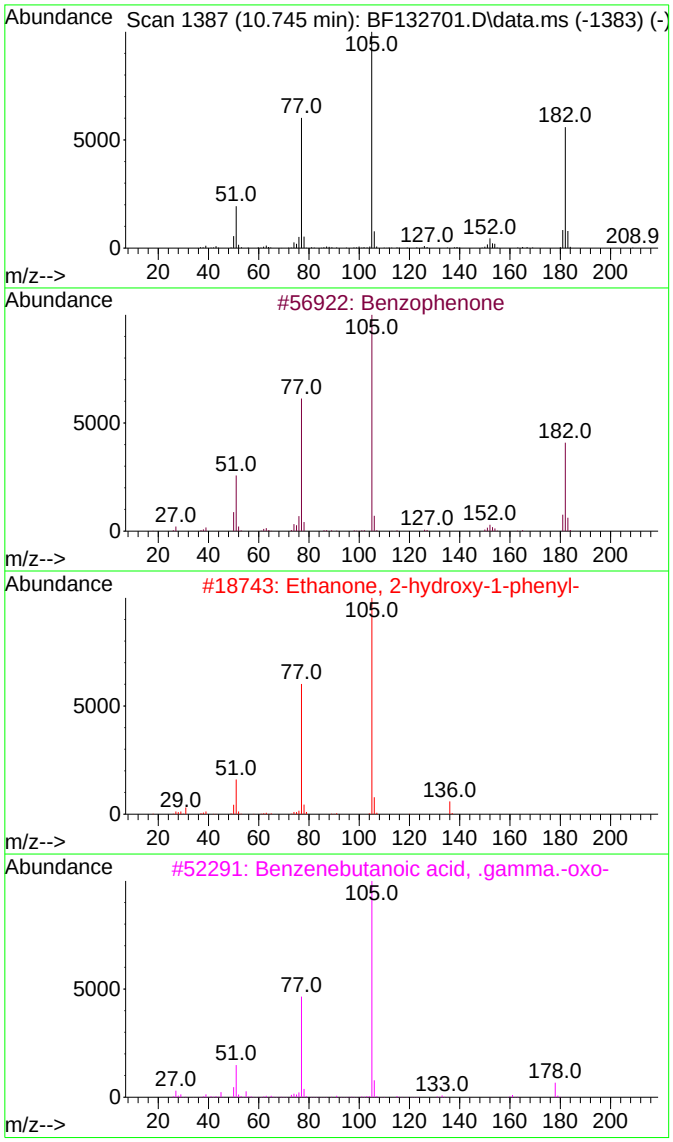
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

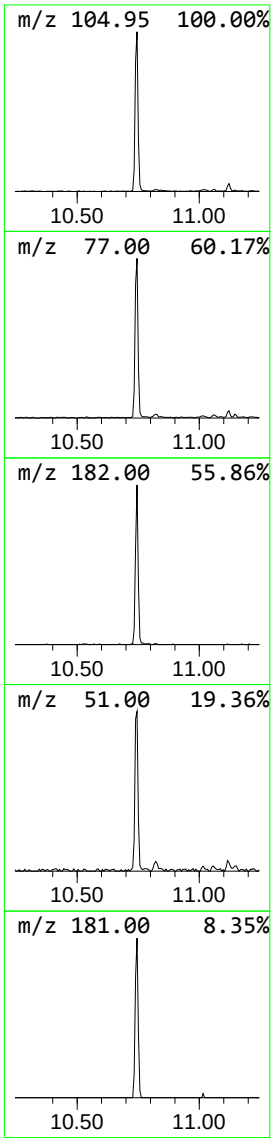
****

Peak Number 2 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.745	4.06 ng	242971	Acenaphthene-d10	10.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Ethanone, 2-hydroxy-1-phenyl-	136	C8H8O2	000582-24-1	47
3	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
4	S-Benzoyl(thiohydroxylamine)	153	C7H7NOS	025740-80-1	47
5	1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47





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Sample : 01829-08
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ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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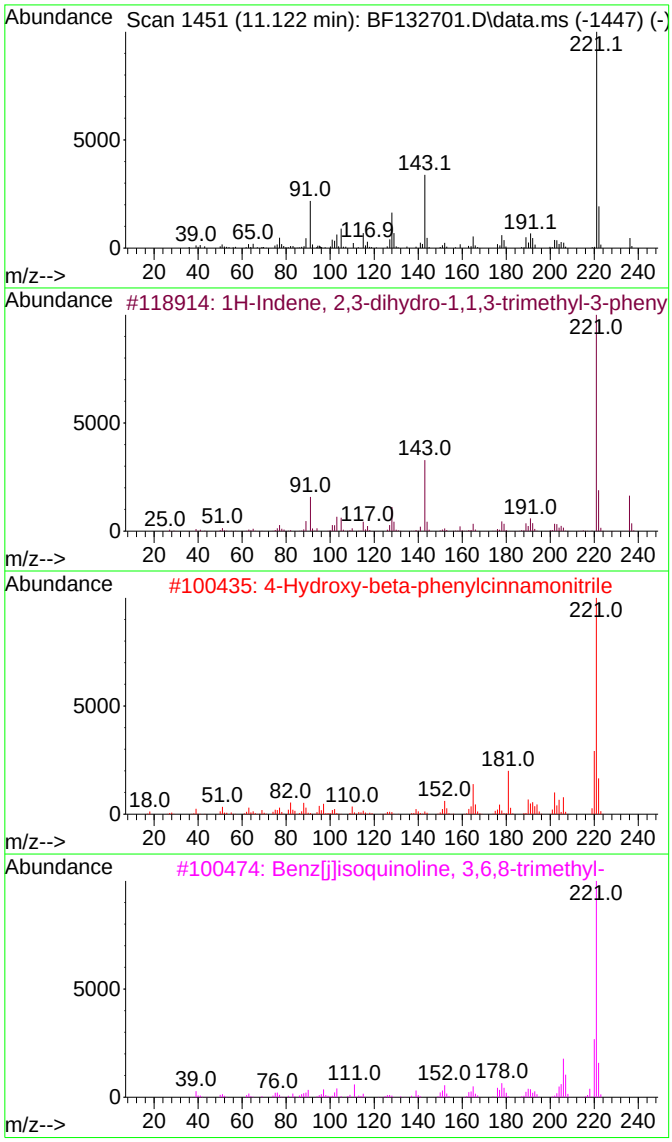
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

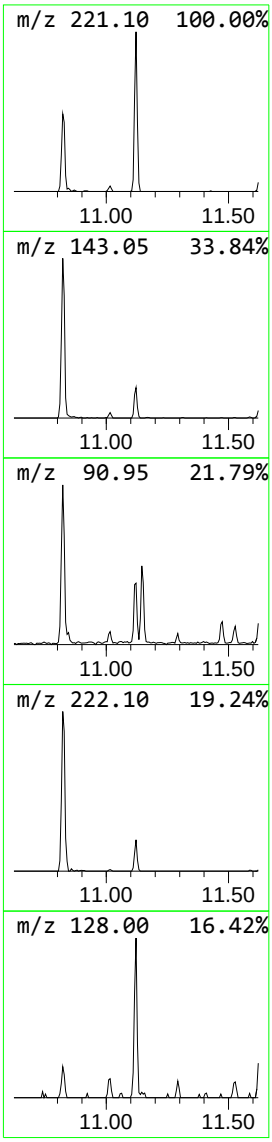
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1H-Indene, 2,3-dihydro-1,1,... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.122	2.58 ng	140644	Phenanthrene-d10	11.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,1,3-tri...	236	C18H20	003910-35-8	86
2	4-Hydroxy-beta-phenylcinnamonitrile	221	C15H11NO	016281-90-6	53
3	Benz[j]isoquinoline, 3,6,8-trime...	221	C16H15N	061171-16-2	50
4	(E)-2-Hydroxy-4'-cyano-stilbene	221	C15H11NO	1000147-85-5	45
5	2-Mercapto-4,6-dimethylnicotinon...	236	C11H16N2SSi	1000332-43-1	40





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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

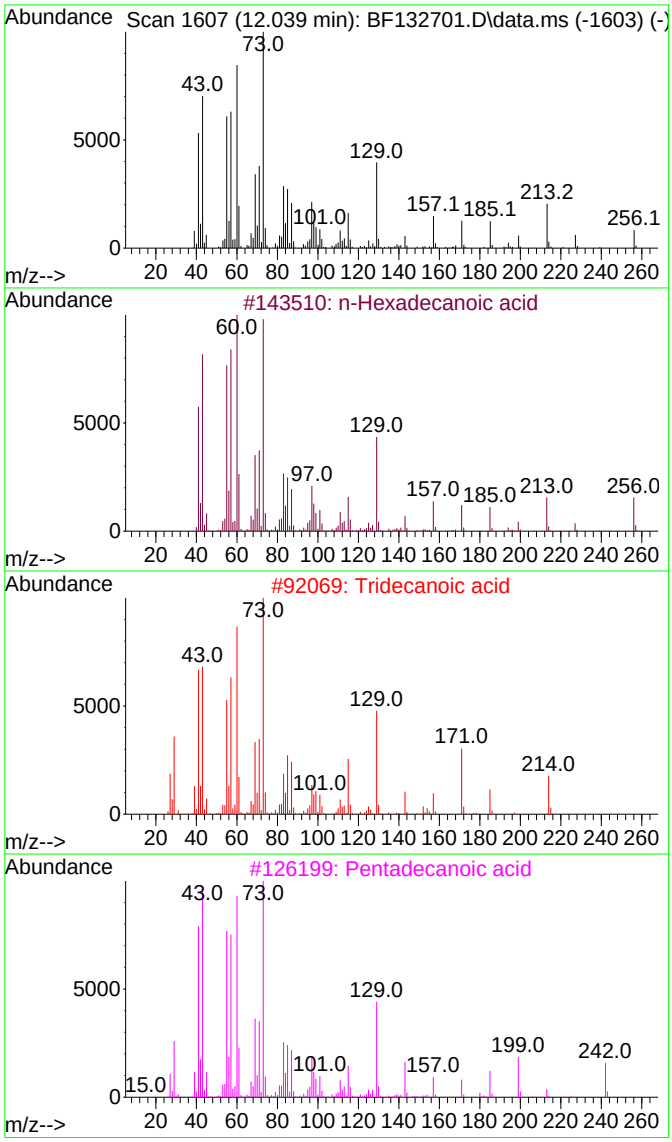
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

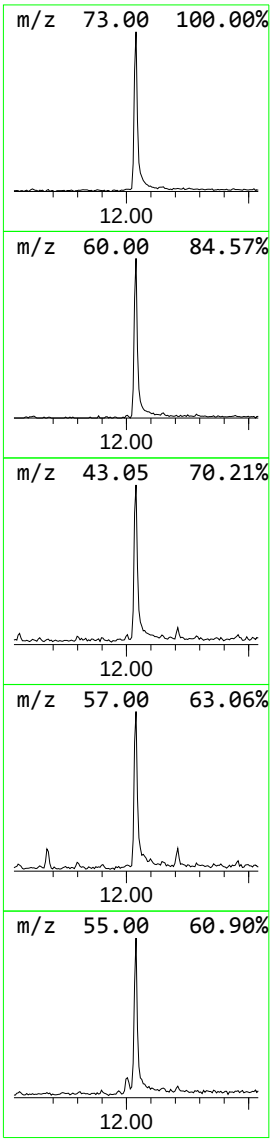
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.039	6.89 ng	375984	Phenanthrene-d10	11.527

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	96
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
5	Dodecanoic acid	200	C12H24O2	000143-07-7	72





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Data File : BF132701.D
Acq On : 08 Mar 2023 21:04
Operator : CG\JU
Sample : 01829-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-08-20230306

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

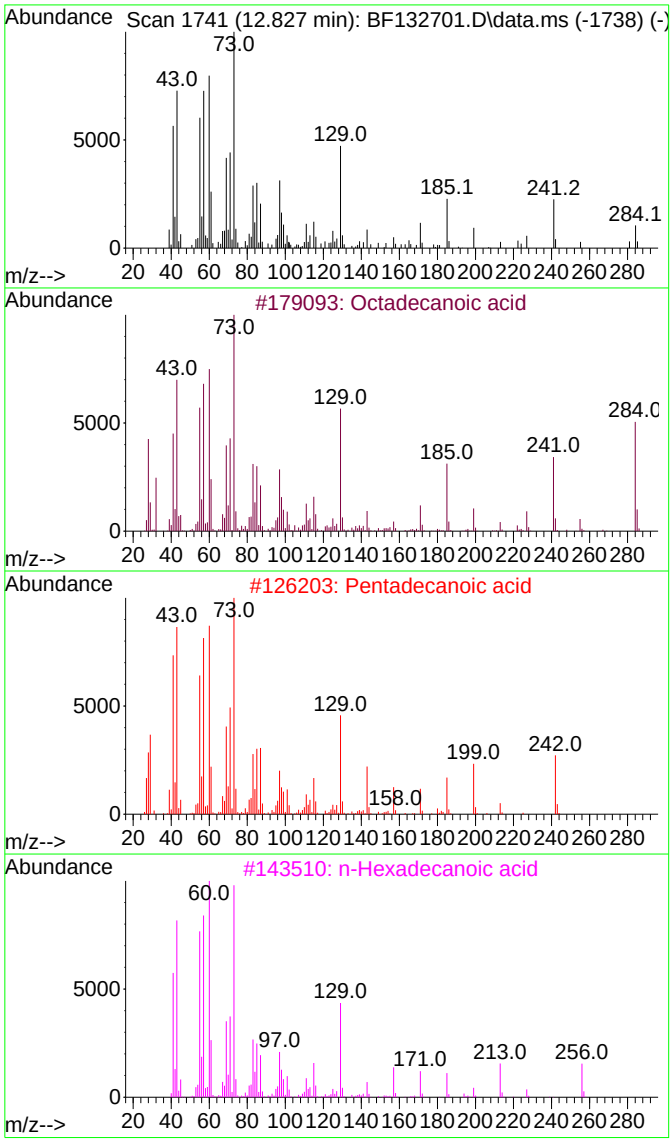
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

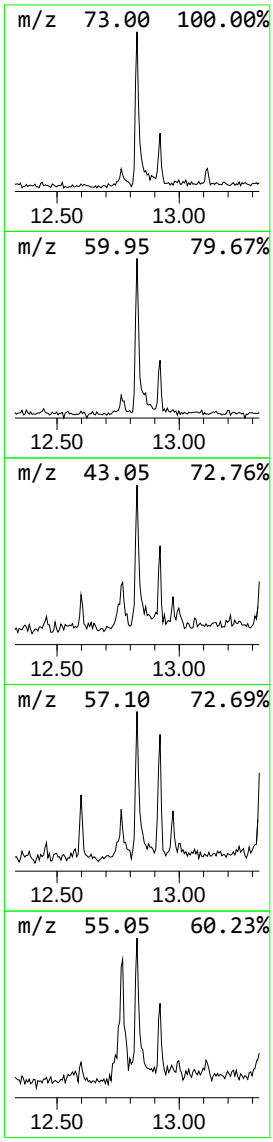
****

Peak Number 5 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.827	2.53 ng	137898	Phenanthrene-d10	11.527

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	89
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

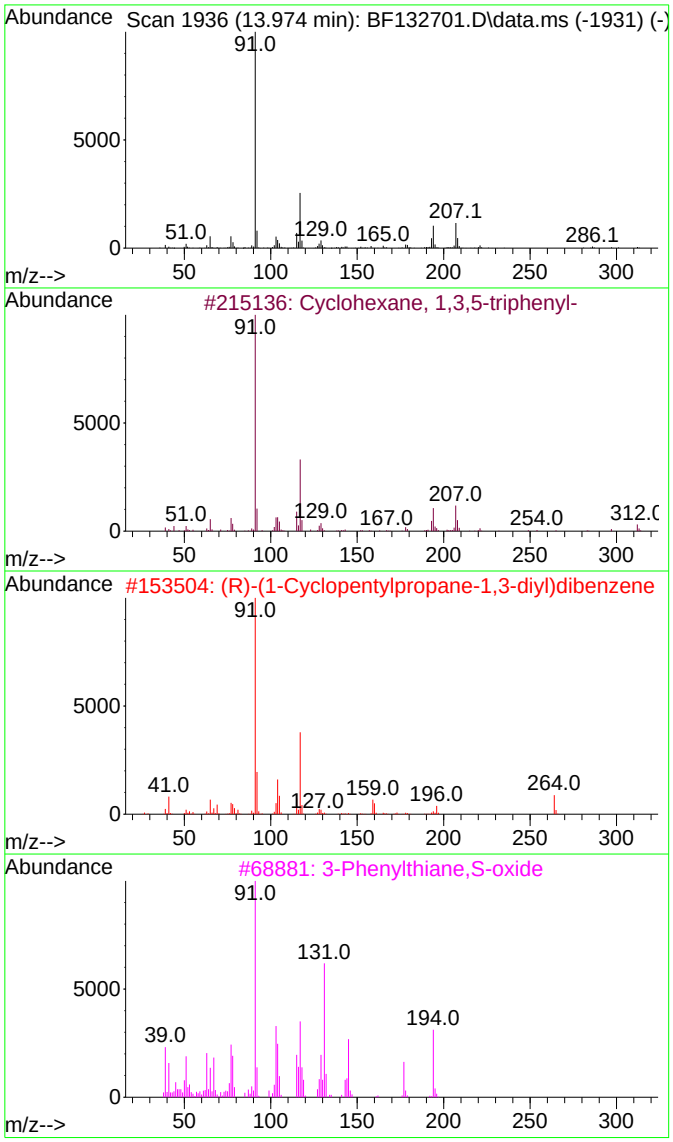
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

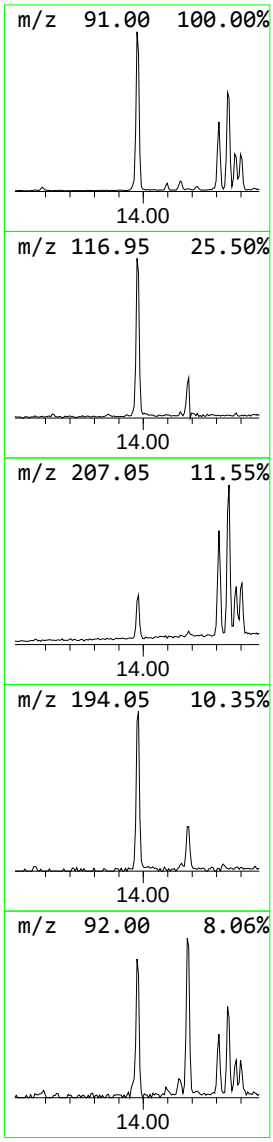
****

Peak Number 6 Cyclohexane, 1,3,5-triphenyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.974	6.91 ng	335522	Chrysene-d12	14.186

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,3,5-triphenyl-	312	C24H24	028336-57-4	83
2	(R)-(1-Cyclopentylpropane-1,3-di...	264	C20H24	1402851-74-4	25
3	3-Phenylthiane,S-oxide	194	C11H14OS	058121-26-9	12
4	(2,3-Diphenylcyclopropyl)methyl ...	332	C22H20OS	131758-71-9	12
5	Benzonitrile, m-phenethyl-	207	C15H13N	034176-91-5	12





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ClientSampleId :
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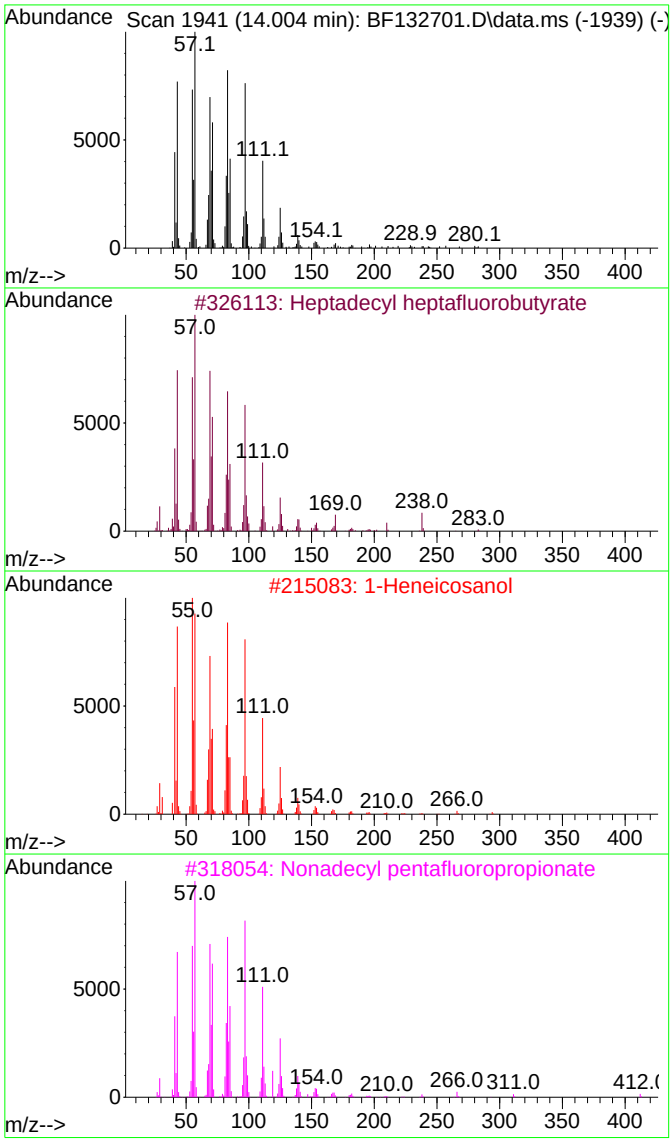
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

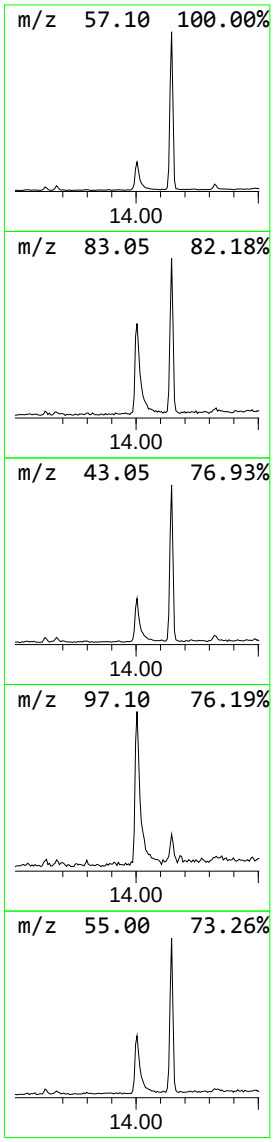
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Heptadecyl heptafluorobutyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.004	9.77 ng	474430	Chrysene-d12	14.186

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
4	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
5	1-Hexacosanol	382	C26H54O	000506-52-5	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030823\
Data File : BF132701.D
Acq On : 08 Mar 2023 21:04
Operator : CG\JU
Sample : 01829-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-08-20230306

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

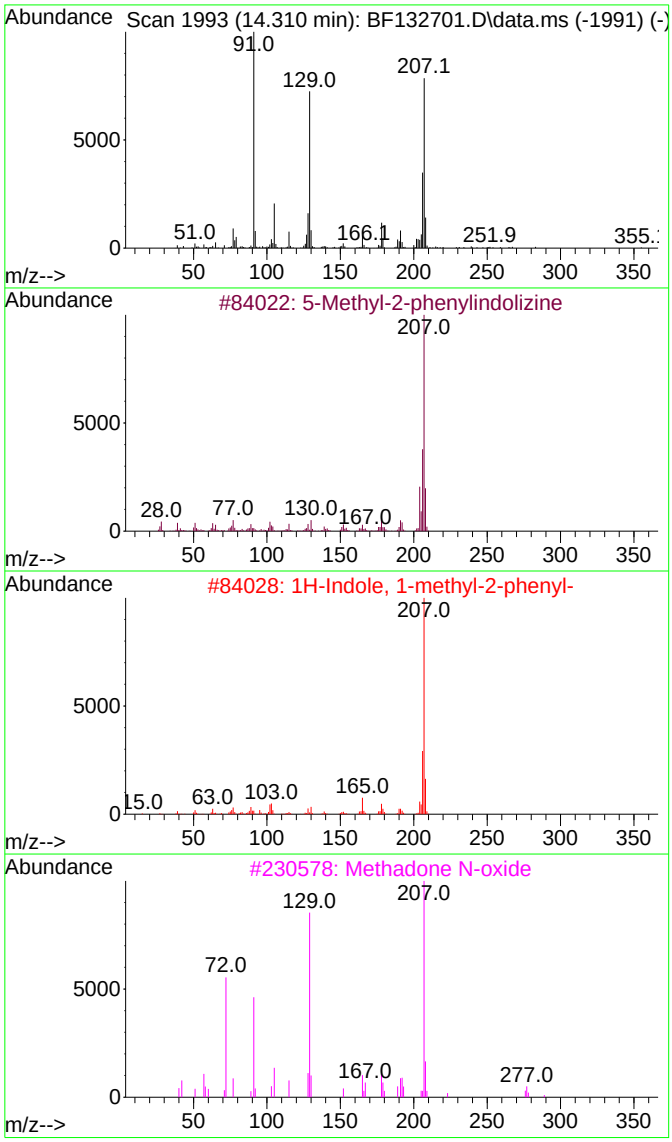
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

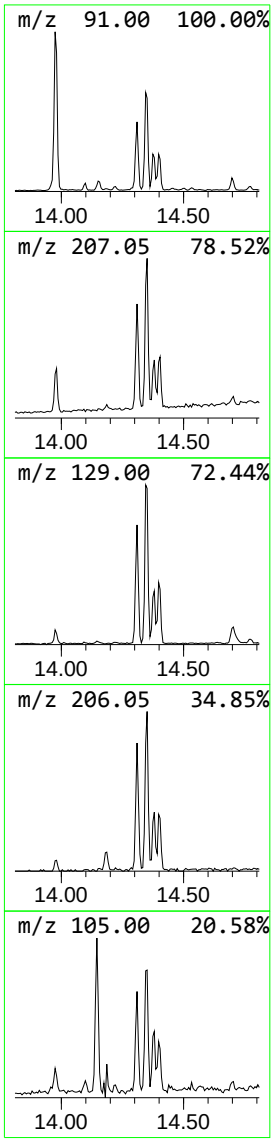
****

Peak Number 8 5-Methyl-2-phenylindolizine Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.310	4.73 ng	229584	Chrysene-d12	14.186

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	55
2	1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	55
3	Methadone N-oxide	325	C21H27NO2	1000120-80-7	53
4	(2,3-Diphenylcyclopropyl)methyl ...	332	C22H20OS	131758-71-9	47
5	Benzo[h]quinoline, 2,4-dimethyl-	207	C15H13N	000605-67-4	46





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Acq On : 08 Mar 2023 21:04
Operator : CG\JU
Sample : 01829-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-08-20230306

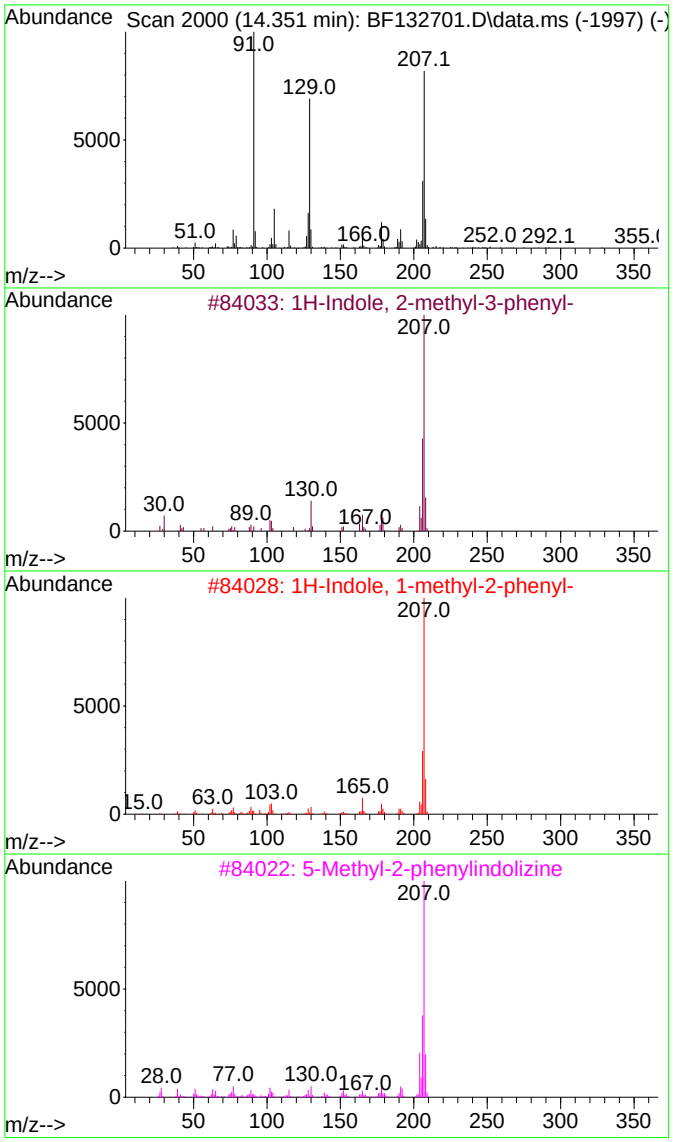
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

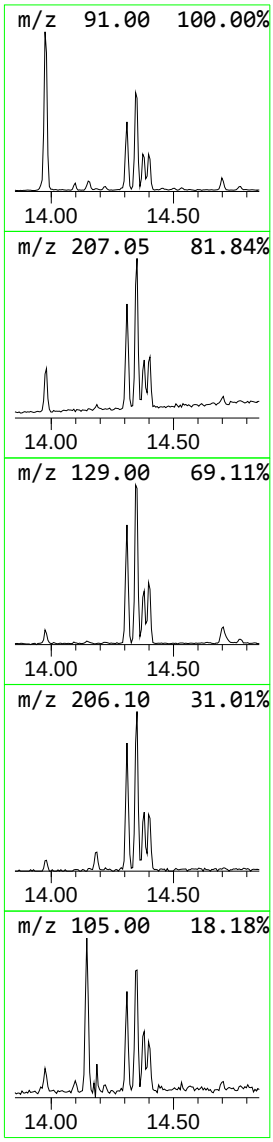
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1H-Indole, 2-methyl-3-phenyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.351	6.49 ng	315419	Chrysene-d12	14.186

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	53
2	1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	53
3	5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	49
4	1-benzylindole	207	C15H13N	1000334-31-3	49
5	7-Methyl -2-phenyl-1H-indole	207	C15H13N	059541-82-1	47





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Data File : BF132701.D
Acq On : 08 Mar 2023 21:04
Operator : CG\JU
Sample : 01829-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-08-20230306

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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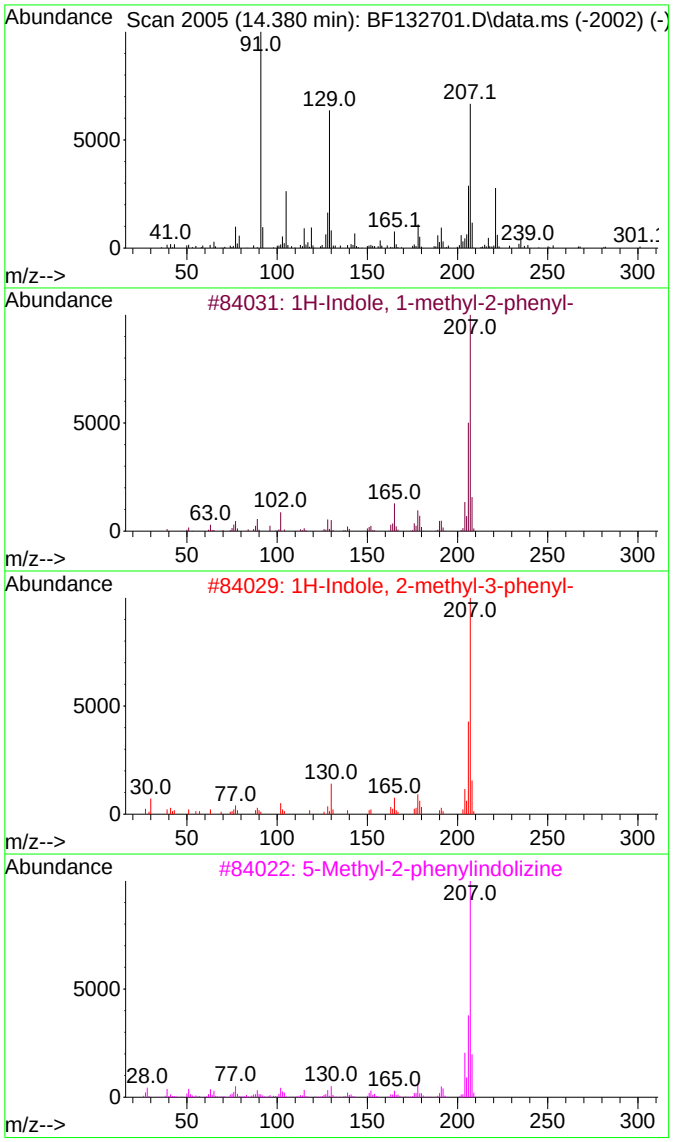
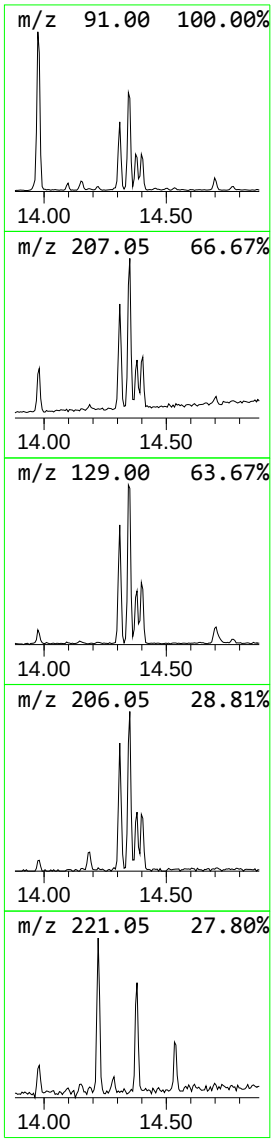
Peak Number 10 unknown14.380 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.380	2.63 ng	127753	Chrysene-d12	14.186

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	45
2	1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	45
3	5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	45
4	9,10-Methanoanthracen-11-ol, 9,1...	250	C18H18O	126615-74-5	30
5	Benzo[h]quinoline, 2,4-dimethyl-	207	C15H13N	000605-67-4	30





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Acq On : 08 Mar 2023 21:04
Operator : CG\JU
Sample : 01829-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SS-08-20230306

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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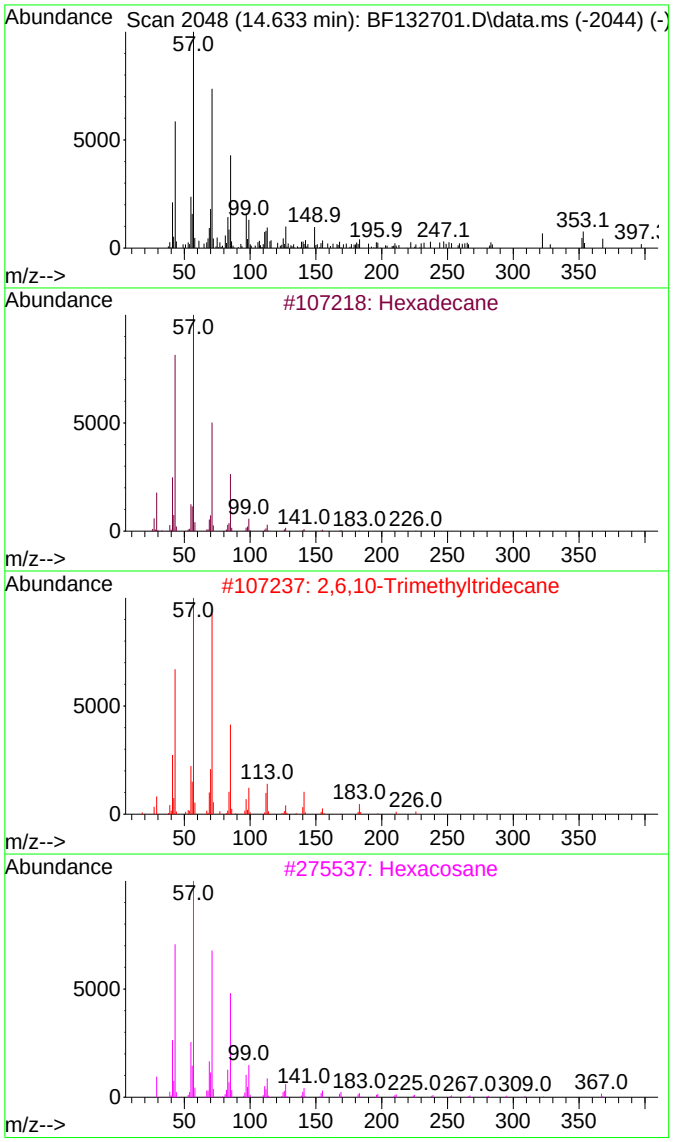
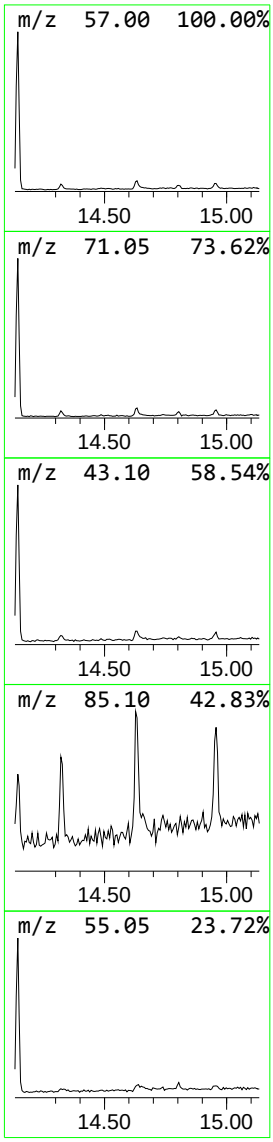
Peak Number 11 Hexadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.633	2.33 ng	113240	Chrysene-d12	14.186

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	93
2	2,6,10-Trimethyltridecane	226	C16H34	003891-99-4	90
3	Hexacosane	366	C26H54	000630-01-3	74
4	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	74
5	Hentriacontane	437	C31H64	000630-04-6	74





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Data File : BF132701.D
Acq On : 08 Mar 2023 21:04
Operator : CG\JU
Sample : 01829-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-08-20230306

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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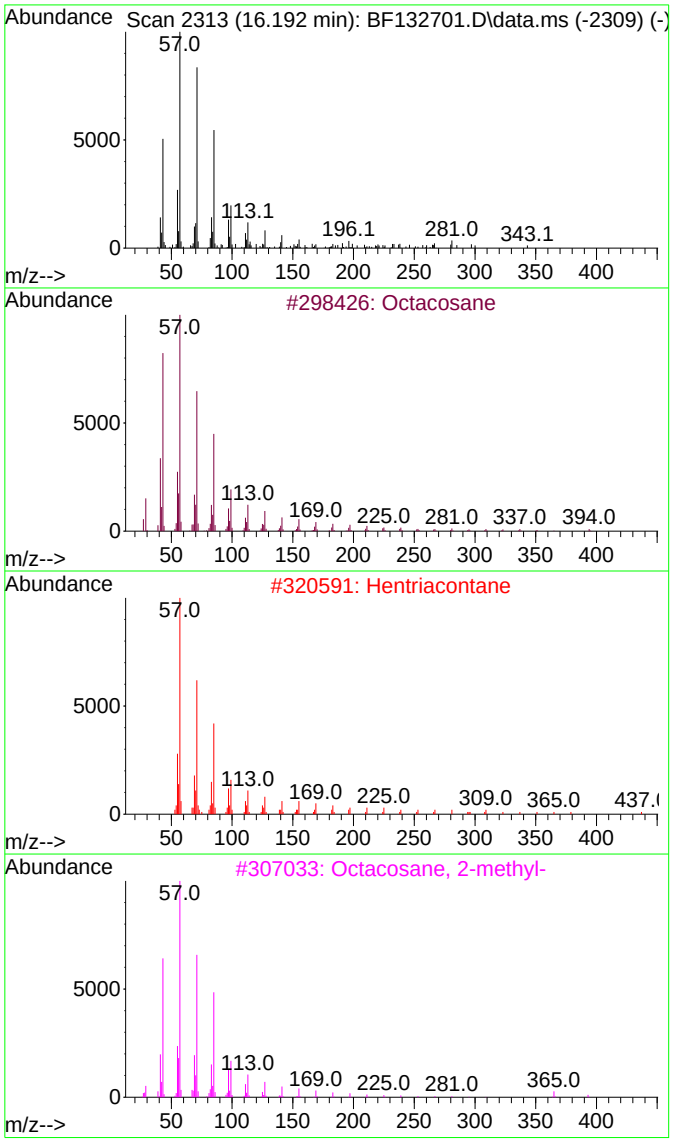
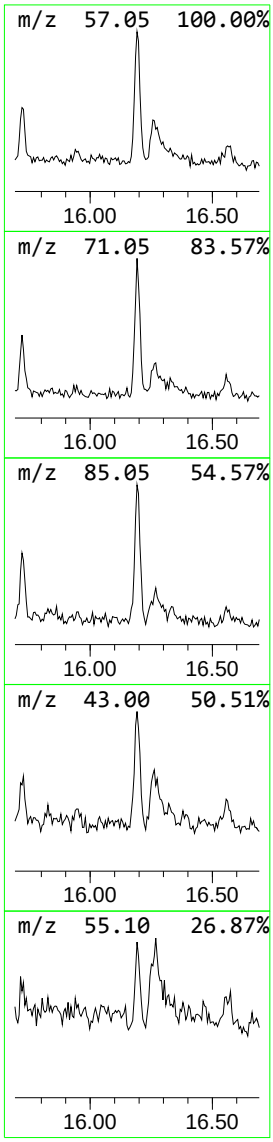
Peak Number 12 Octacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.192	2.32 ng	117675	Perylene-d12	15.727

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Hentriacontane	437	C31H64	000630-04-6	90
3	Octacosane, 2-methyl-	408	C29H60	001560-98-1	86
4	Eicosane	282	C20H42	000112-95-8	86
5	Heneicosane	296	C21H44	000629-94-7	86





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Acq On : 08 Mar 2023 21:04
Operator : CG\JU
Sample : 01829-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-08-20230306

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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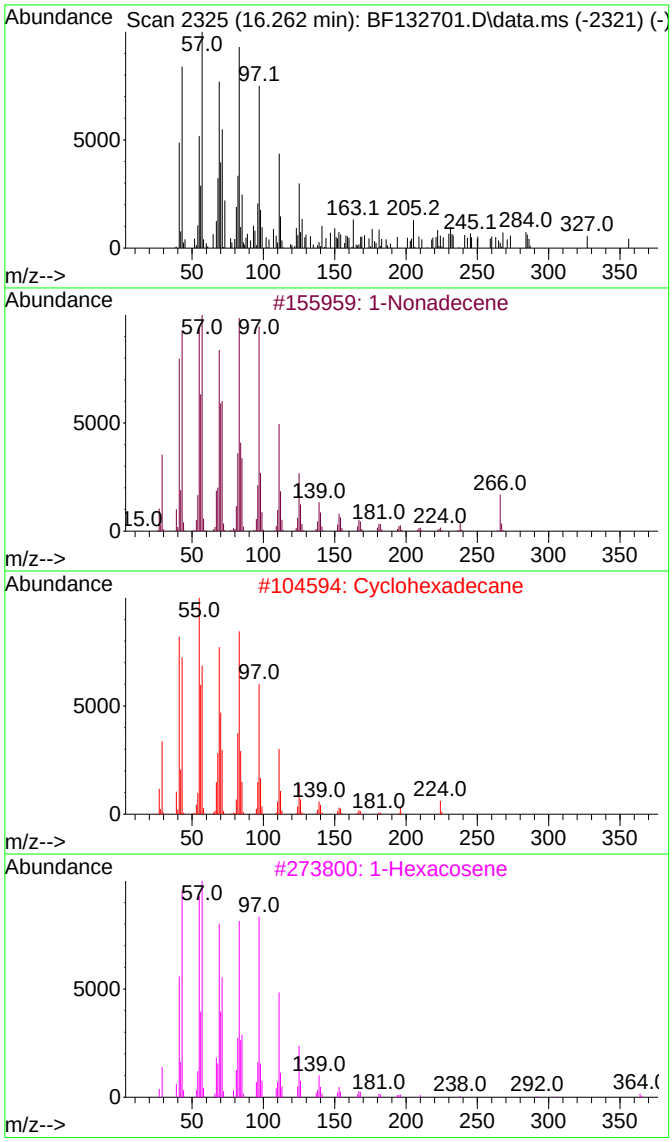
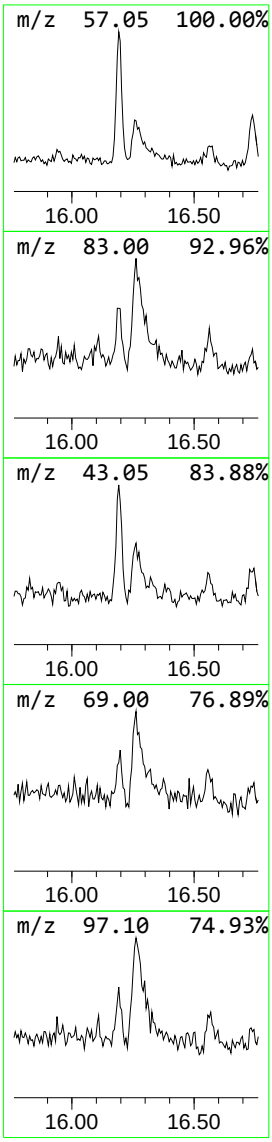
Peak Number 13 1-Nonadecene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.262	2.15 ng	109121	Perylene-d12	15.727

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	93
2	Cyclohexadecane	224	C16H32	000295-65-8	90
3	1-Hexacosene	364	C26H52	018835-33-1	87
4	1-Hexacosanol	382	C26H54O	000506-52-5	87
5	5-Fluoro-3-trifluoromethylbenzoi...	474	C27H42F4O2	1000338-91-1	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030823\
Data File : BF132701.D
Acq On : 08 Mar 2023 21:04
Operator : CG\JU
Sample : 01829-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-08-20230306

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-...	5.222	32.6	ng	1479170	1	6.987	907457	20.0
Benzophenone	10.745	4.1	ng	242971	3	10.033	1197800	20.0
1H-Indene, 2,3-...	11.122	2.6	ng	140644	4	11.527	1090610	20.0
n-Hexadecanoic ...	12.039	6.9	ng	375984	4	11.527	1090610	20.0
Octadecanoic acid	12.827	2.5	ng	137898	4	11.527	1090610	20.0
Cyclohexane, 1,...	13.974	6.9	ng	335522	5	14.186	971279	20.0
Heptadecyl hept...	14.004	9.8	ng	474430	5	14.186	971279	20.0
5-Methyl-2-phen...	14.310	4.7	ng	229584	5	14.186	971279	20.0
1H-Indole, 2-me...	14.351	6.5	ng	315419	5	14.186	971279	20.0
unknown14.380	14.380	2.6	ng	127753	5	14.186	971279	20.0
Hexadecane	14.633	2.3	ng	113240	5	14.186	971279	20.0
Octacosane	16.192	2.3	ng	117675	6	15.727	1012830	20.0
1-Nonadecene	16.262	2.1	ng	109121	6	15.727	1012830	20.0