LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071923\
Data File : BF134369.D
Acq On : 19 Jul 2023 20:52
Operator : CG\JU
Sample : 03641-11
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP14

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-BF062623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134369.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	7	19	25	rVB	218829	316260	13.13%	2.111%
2	5.110	510	514	522	rVB	35785	50438	2.09%	0.337%
3	5.487	573	578	581	rBV	2139016	2001613	83.11%	13.363%
4	6.487	742	748	765	rBV	1909206	2077228	86.25%	13.867%
5	6.834	804	807	813	rBV	483910	442513	18.37%	2.954%
6	7.404	899	904	907	rBV	1423326	1292449	53.66%	8.628%
7	8.116	1021	1025	1028	rBV	703673	554826	23.04%	3.704%
8	9.192	1204	1208	1211	rBV	2834605	2408478	100.00%	16.079%
9	9.875	1320	1324	1327	rBV	678195	571344	23.72%	3.814%
10	10.669	1455	1459	1462	rBV	1647054	1404525	58.32%	9.377%
11	11.369	1574	1578	1581	rBV	631579	508403	21.11%	3.394%
12	11.898	1665	1668	1672	rBV	188208	164432	6.83%	1.098%
13	12.592	1782	1786	1789	rBV	66185	66878	2.78%	0.446%
14	12.686	1800	1802	1808	rBV	33555	42090	1.75%	0.281%
15	12.821	1820	1825	1829	rVB	56567	55096	2.29%	0.368%
16	12.969	1845	1850	1853	rBV	2161323	1897741	78.79%	12.669%
17	13.898	2005	2008	2022	rVB4	41170	90406	3.75%	0.604%
18	14.027	2026	2030	2034	rBV	403608	423969	17.60%	2.830%
19	14.121	2043	2046	2052	rVB2	31074	31346	1.30%	0.209%
20	14.492	2104	2109	2115	rVB3	31266	42919	1.78%	0.287%
21	14.551	2115	2119	2124	rBV7	15041	27063	1.12%	0.181%
22	14.963	2185	2189	2192	rVB2	34877	36689	1.52%	0.245%
23	15.092	2207	2211	2215	rBV	25273	43432	1.80%	0.290%
24	15.157	2218	2222	2226	rBV	31606	39332	1.63%	0.263%
25	15.533	2281	2286	2298	rBV	247942	340729	14.15%	2.275%
26	16.009	2363	2367	2373	rVB2	30563	48969	2.03%	0.327%

Sum of corrected areas: 14979168

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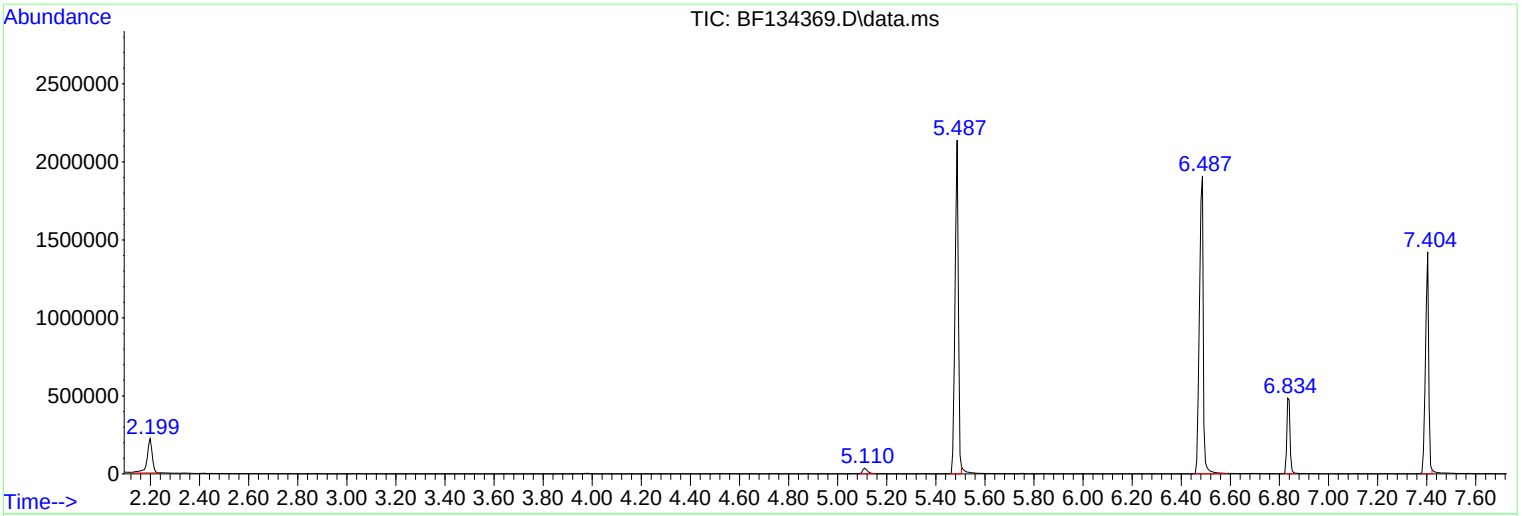
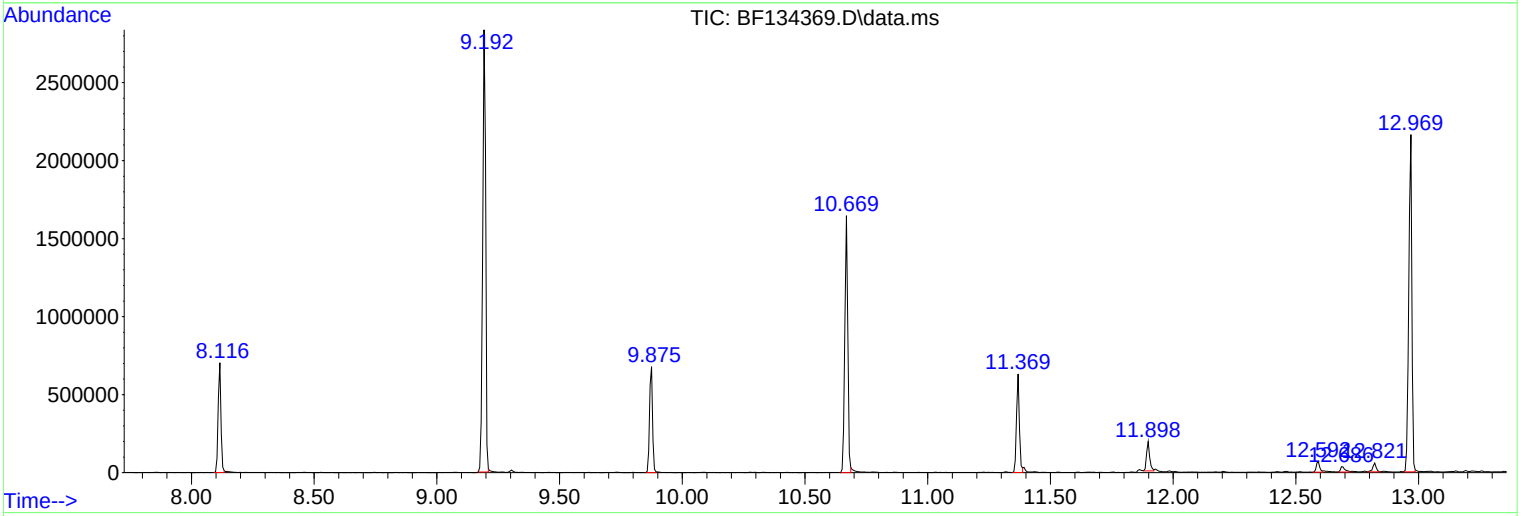
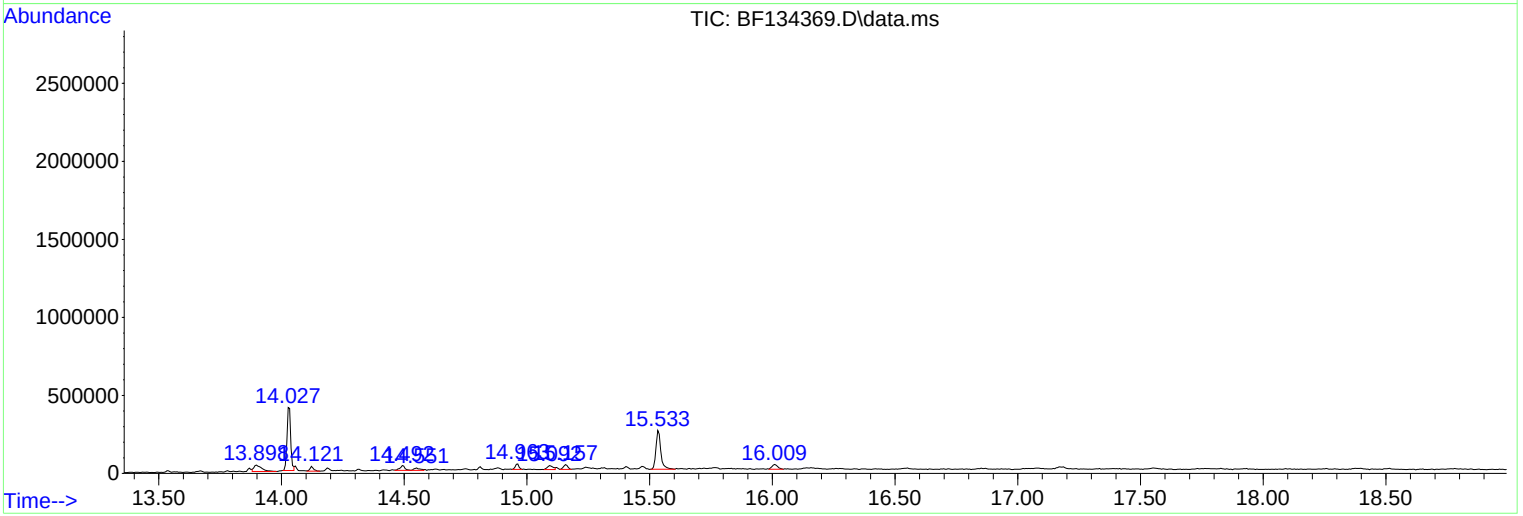
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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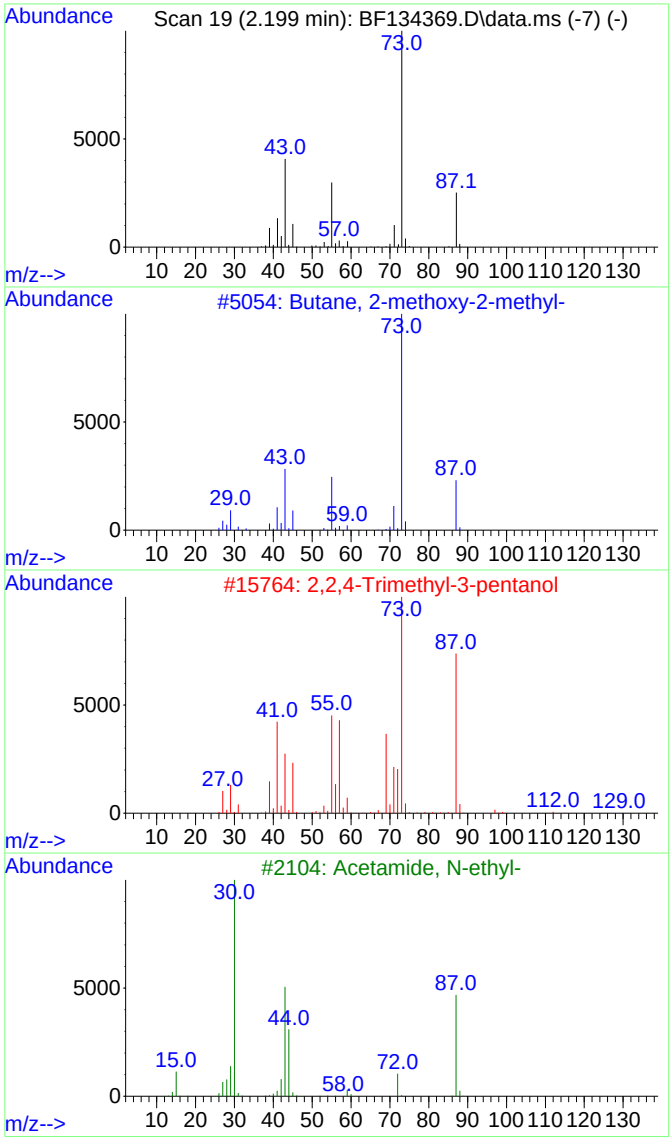
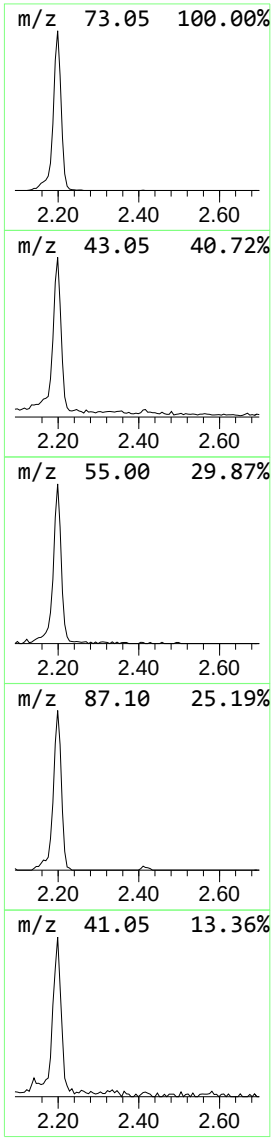
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.199	14.29 ng	316260	1,4-Dichlorobenzene-d4	6.840

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4	Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	17
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12





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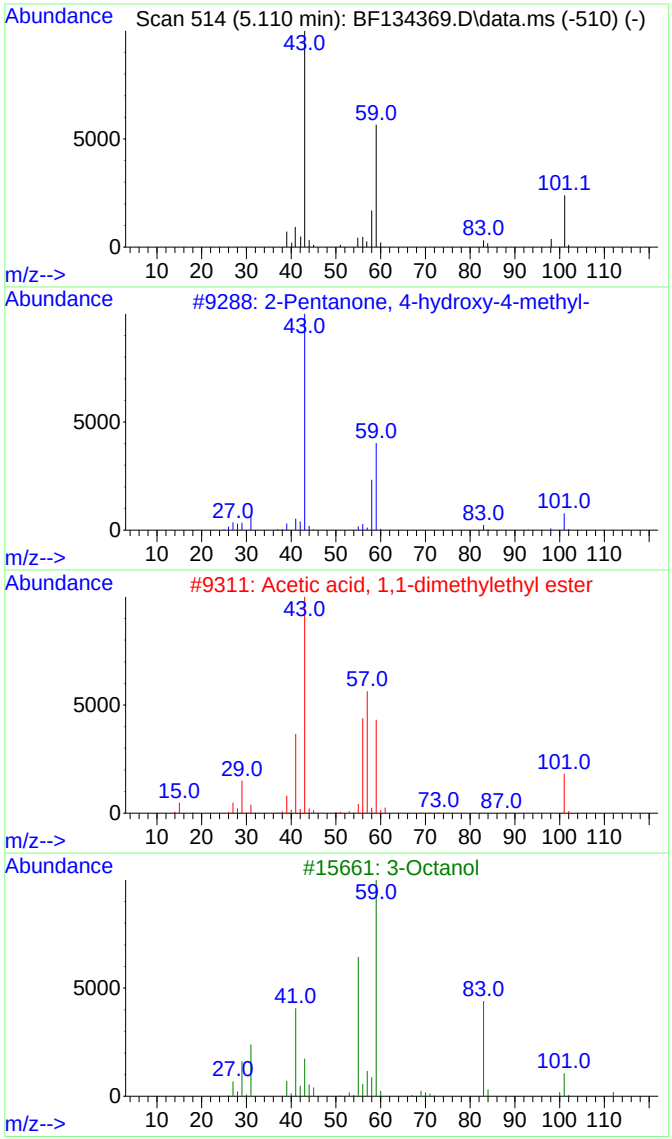
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

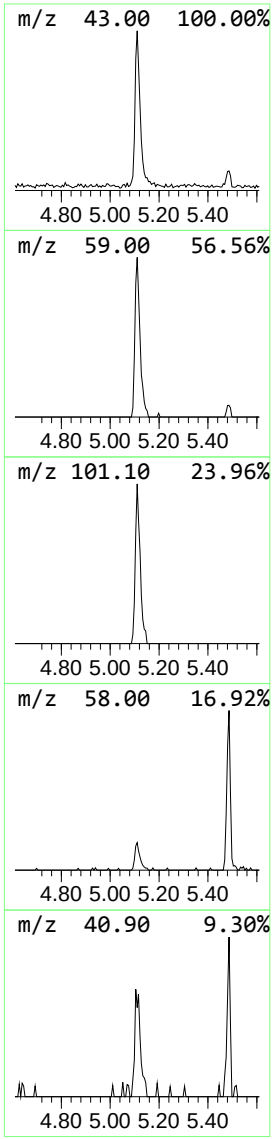
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	2.28 ng	50438	1,4-Dichlorobenzene-d4	6.840

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Octanol	130	C8H18O	000589-98-0	23
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9





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Sample : 03641-11
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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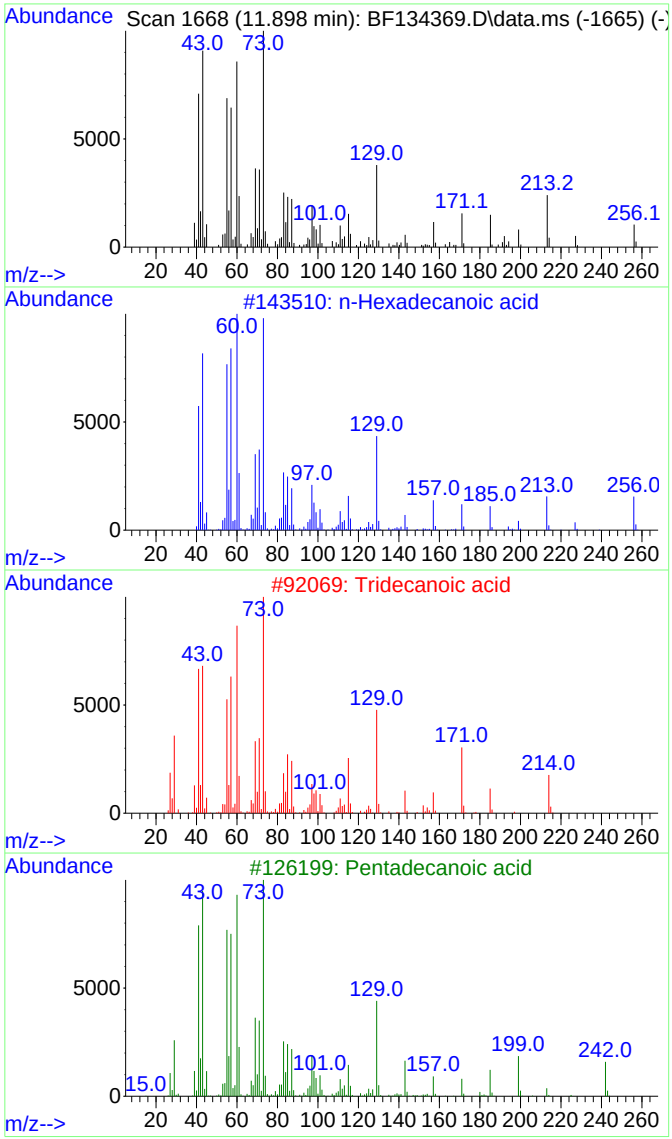
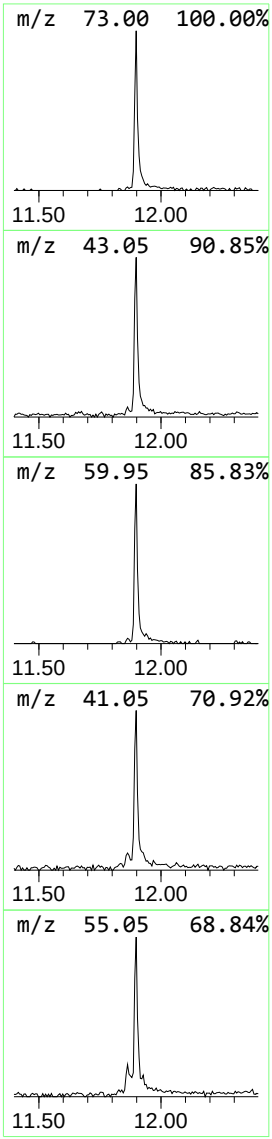
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	6.47 ng	164432	Phenanthrene-d10	11.369

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	97
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	n-Decanoic acid	172	C10H20O2	000334-48-5	70
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	68





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BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

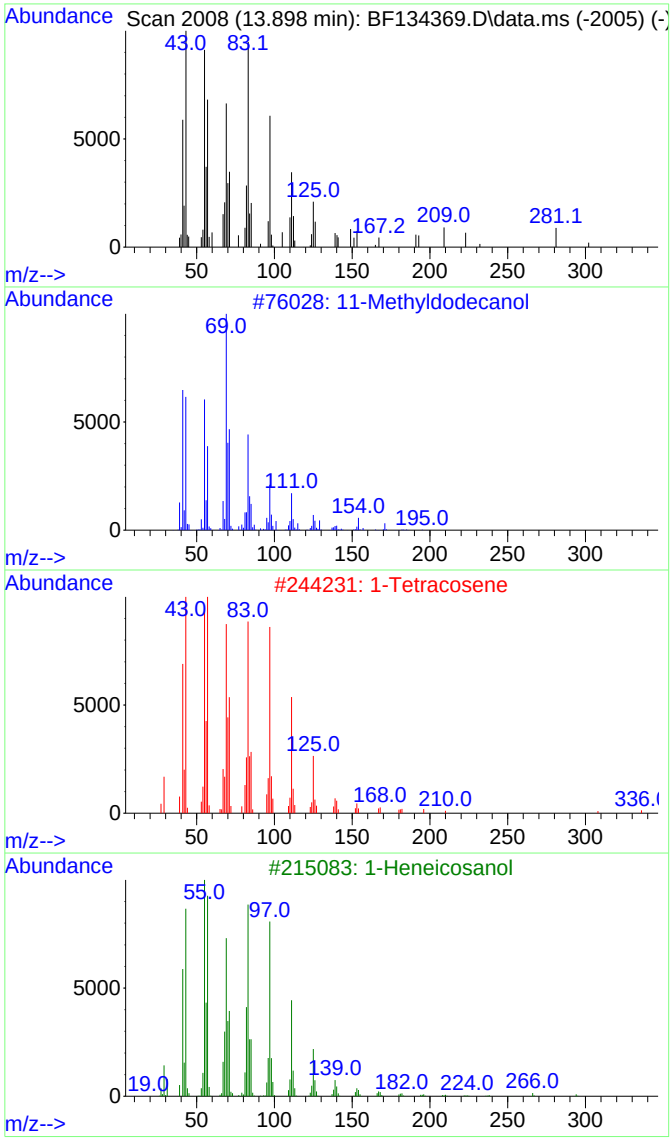
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

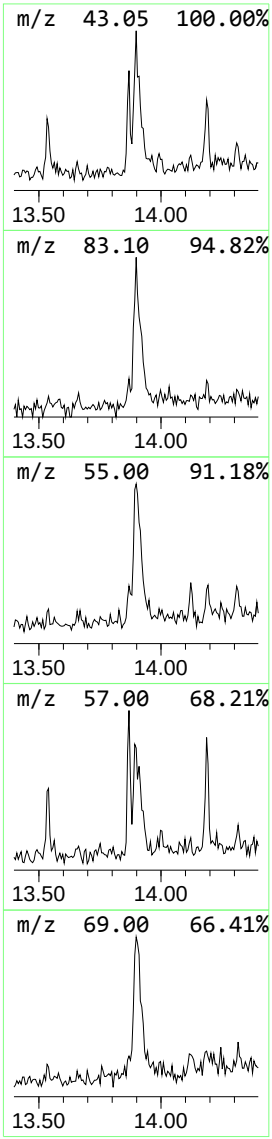
****

Peak Number 5 11-Methyldodecanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	4.26 ng	90406	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Methyldodecanol	200	C13H28O	085763-57-1	80
2	1-Tetracosene	336	C24H48	010192-32-2	64
3	1-Heneicosanol	312	C21H44O	015594-90-8	60
4	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	58
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	58





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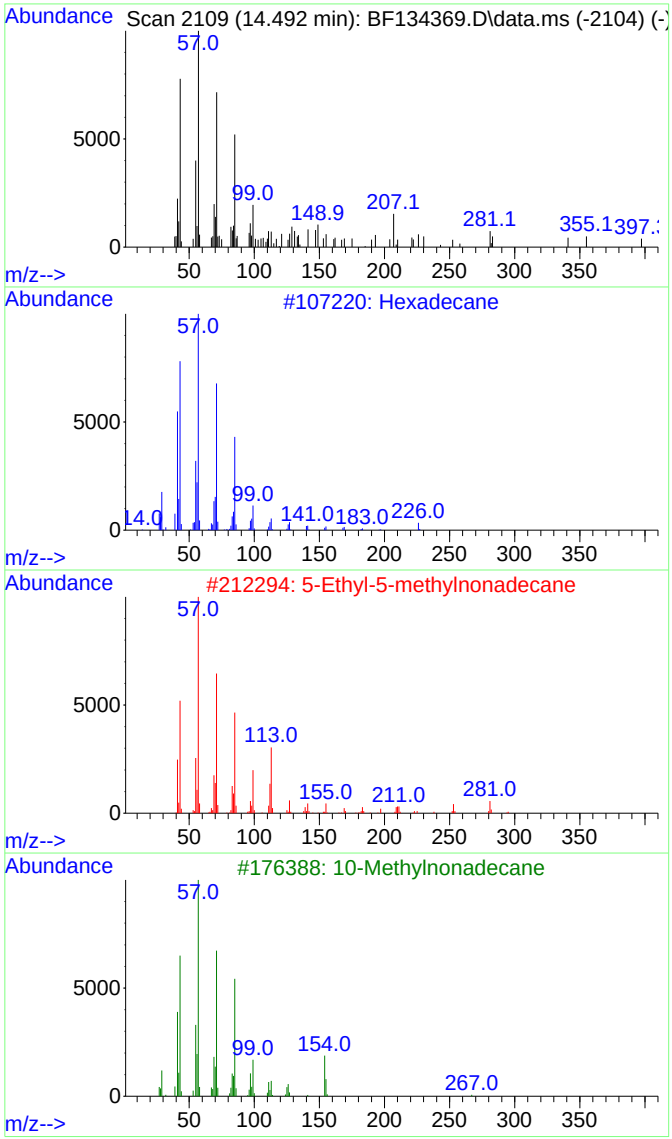
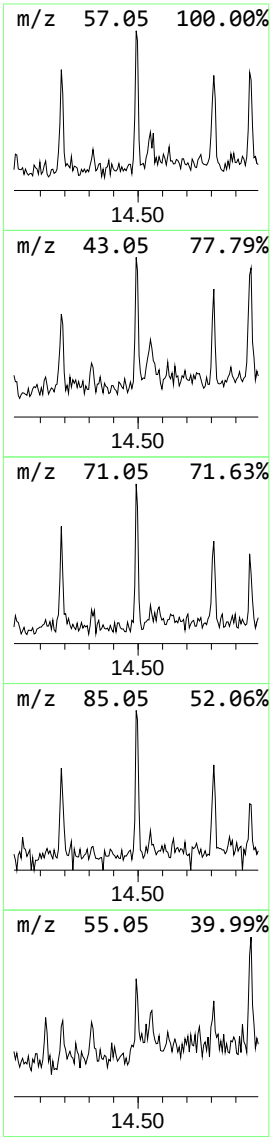
****

Peak Number 6 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.492	2.02 ng	42919	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	83
2	5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	74
3	10-Methylnonadecane	282	C20H42	056862-62-5	68
4	Heptadecane	240	C17H36	000629-78-7	64
5	Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	64





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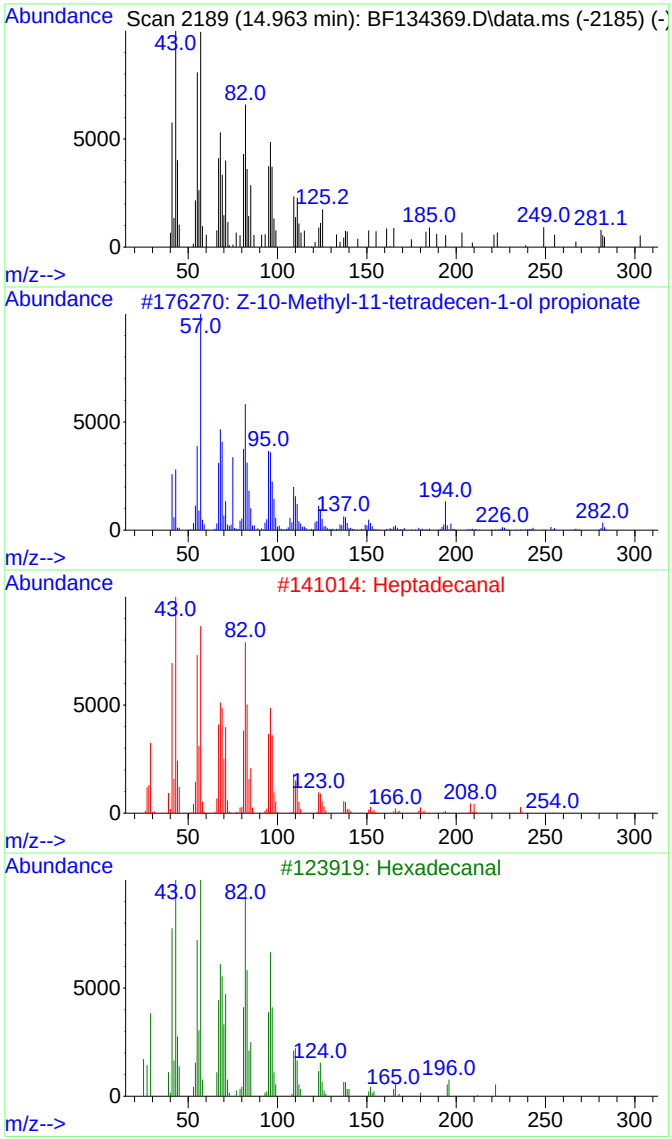
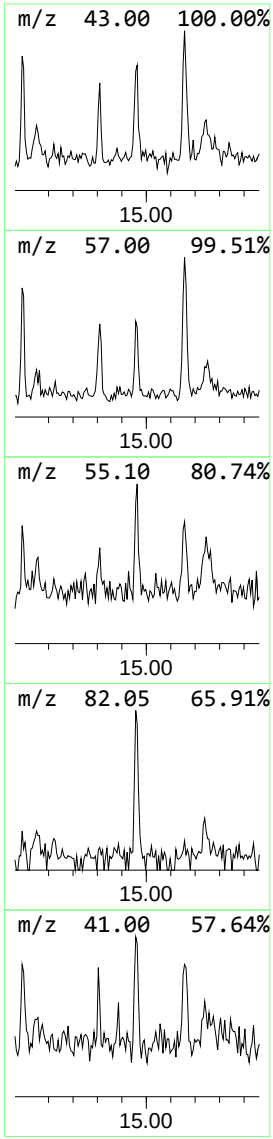
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Z-10-Methyl-11-tetradecen-1... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.963	2.15 ng	36689	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Z-10-Methyl-11-tetradecen-1-ol p...	282	C18H34O2	1000130-77-5	90
2	Heptadecanal	254	C17H34O	1000376-70-0	87
3	Hexadecanal	240	C16H32O	000629-80-1	83
4	Pentadecanal-	226	C15H30O	002765-11-9	80
5	Tridecanal	198	C13H26O	010486-19-8	74





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TIC Library : C:\Database\NIST20.L
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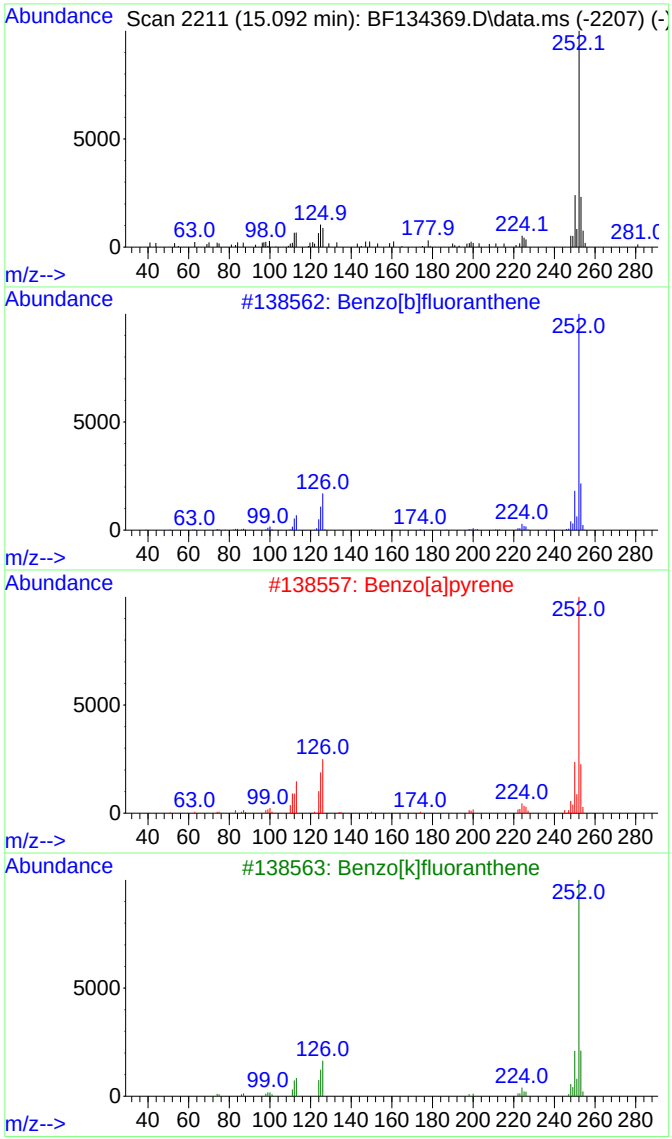
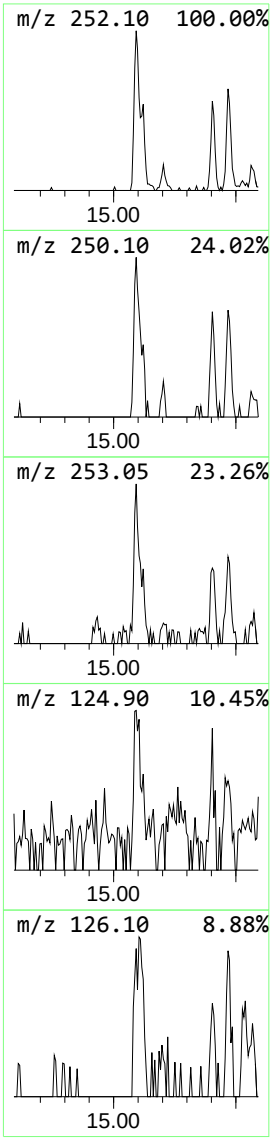
Peak Number 8 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.092	2.55 ng	43432	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]fluoranthene	252	C20H12	000205-99-2	91
2	Benzo[a]pyrene	252	C20H12	000050-32-8	90
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	90
4	Benzo[e]pyrene	252	C20H12	000192-97-2	81
5	Perylene	252	C20H12	000198-55-0	76





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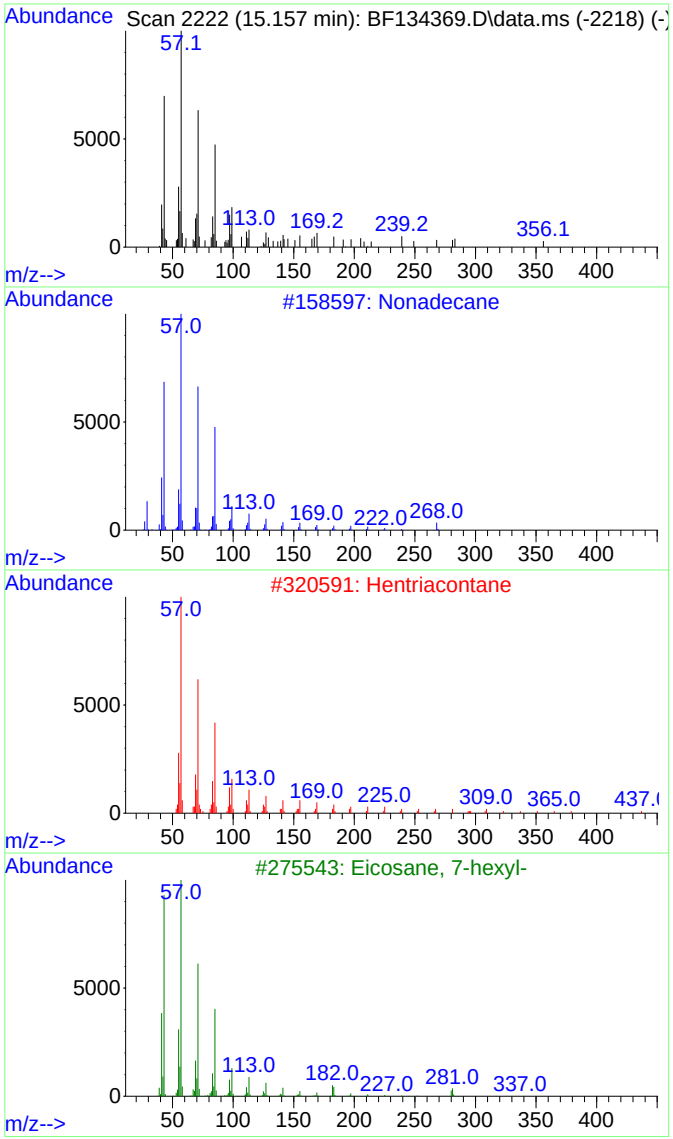
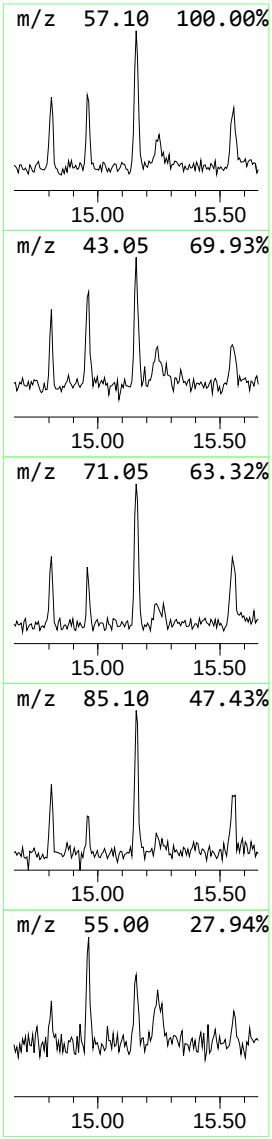
Peak Number 9 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.157	2.31 ng	39332	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	95
2	Hentriacontane	437	C31H64	000630-04-6	87
3	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	86
4	Heptadecane	240	C17H36	000629-78-7	83
5	Tetracosane	338	C24H50	000646-31-1	83





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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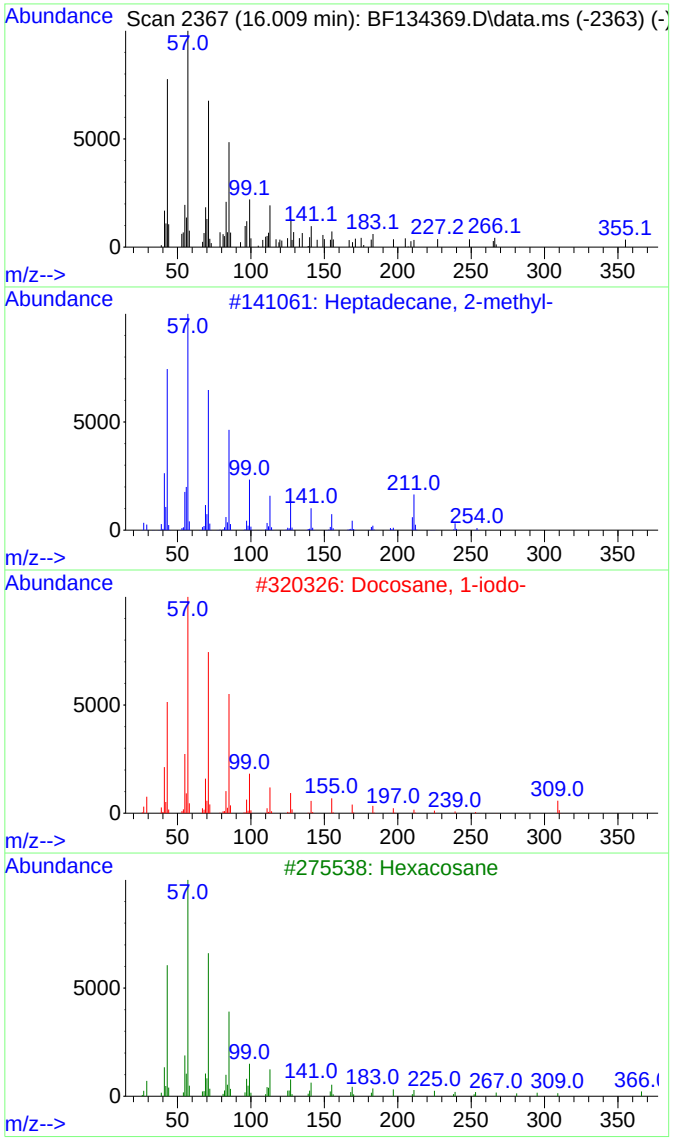
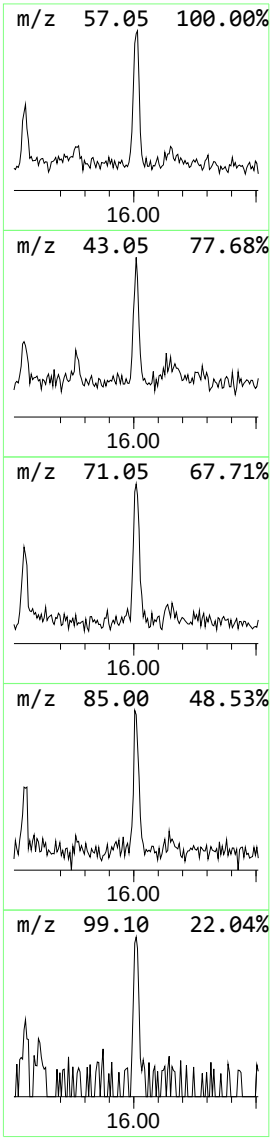
Peak Number 10 Heptadecane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.009	2.87 ng	48969	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	80
2	Docosane, 1-iodo-	436	C22H45I	1000406-31-9	74
3	Hexacosane	366	C26H54	000630-01-3	74
4	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	74
5	Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	74





Tentatively Identified Compound (LSC) summary

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TP14

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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
Butane, 2-metho...	2.199	14.3	ng	316260	1	6.840	442513	20.0
2-Pentanone, 4-...	5.110	2.3	ng	50438	1	6.840	442513	20.0
n-Hexadecanoic ...	11.898	6.5	ng	164432	4	11.369	508403	20.0
11-Methyldodecanol	13.898	4.3	ng	90406	5	14.033	423969	20.0
Hexadecane	14.492	2.0	ng	42919	5	14.033	423969	20.0
Z-10-Methyl-11-...	14.963	2.1	ng	36689	6	15.533	340729	20.0
Benzo[e]pyrene	15.092	2.5	ng	43432	6	15.533	340729	20.0
Nonadecane	15.157	2.3	ng	39332	6	15.533	340729	20.0
Heptadecane, 2-...	16.009	2.9	ng	48969	6	15.533	340729	20.0