LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091823\
Data File : BF135317.D
Acq On : 18 Sep 2023 20:48
Operator : CG\JU
Sample : 04399-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11985

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-BF091123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135317.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	7	11	26	rVB2	24176	50203	1.46%	0.175%
2	5.004	492	496	504	rBV	53489	75312	2.19%	0.263%
3	5.393	558	562	574	rBV	2972420	3176348	92.28%	11.077%
4	6.404	729	734	737	rBV	3032604	3156783	91.71%	11.009%
5	6.757	790	794	797	rBV	1097001	882772	25.65%	3.079%
6	7.322	885	890	893	rBV	2201294	2089014	60.69%	7.285%
7	8.034	1007	1011	1017	rBV	1358970	1138369	33.07%	3.970%
8	9.116	1189	1195	1198	rBV	3748720	3442026	100.00%	12.004%
9	9.234	1210	1215	1218	rVB	36274	36565	1.06%	0.128%
10	9.792	1306	1310	1313	rBV	1444598	1189172	34.55%	4.147%
11	10.586	1440	1445	1448	rBV	2131944	1935651	56.24%	6.751%
12	11.280	1560	1563	1566	rBV	1218297	1169335	33.97%	4.078%
13	11.304	1566	1567	1571	rVV	405927	290178	8.43%	1.012%
14	11.357	1571	1576	1579	rVB	51080	54068	1.57%	0.189%
15	11.522	1598	1604	1609	rBV	39583	49470	1.44%	0.173%
16	11.786	1645	1649	1651	rBV2	74990	70451	2.05%	0.246%
17	11.816	1651	1654	1661	rVV	333735	383941	11.15%	1.339%
18	11.898	1665	1668	1670	rVV	103520	103944	3.02%	0.363%
19	11.922	1670	1672	1678	rVB	44771	41443	1.20%	0.145%
20	12.086	1697	1700	1702	rBV	44431	36994	1.07%	0.129%
21	12.116	1702	1705	1710	rVB	77444	66846	1.94%	0.233%
22	12.427	1755	1758	1762	rBV	42145	42583	1.24%	0.149%
23	12.504	1767	1771	1774	rBV	714050	658094	19.12%	2.295%
24	12.592	1783	1786	1788	rBV2	59011	56612	1.64%	0.197%
25	12.692	1800	1803	1805	rBV2	71060	67122	1.95%	0.234%
26	12.733	1805	1810	1813	rVB	562836	585982	17.02%	2.044%
27	12.880	1831	1835	1838	rBV	2553501	2242550	65.15%	7.821%
28	12.957	1843	1848	1851	rBV4	34113	48411	1.41%	0.169%
29	13.039	1859	1862	1864	rBV2	33741	39994	1.16%	0.139%
30	13.063	1864	1866	1869	rVB	70834	63386	1.84%	0.221%
31	13.133	1869	1878	1880	rBV2	47971	68991	2.00%	0.241%
32	13.169	1880	1884	1887	rVV	46585	47213	1.37%	0.165%
33	13.580	1951	1954	1958	rBV	45435	46293	1.34%	0.161%
34	13.686	1967	1972	1974	rBV	68110	70933	2.06%	0.247%
35	13.786	1987	1989	1992	rBV	52475	44713	1.30%	0.156%
36	13.827	1992	1996	2006	rVB5	52455	144248	4.19%	0.503%

LSC Area Percent Report

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Misc :
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Instrument : BNA_F
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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
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Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.939	2008	2015	2018	rBV3	830442	1187924	34.51%	4.143%
38	13.963	2018	2019	2025	rVB	286728	215763	6.27%	0.752%
39	14.045	2030	2033	2035	rVB	41768	39392	1.14%	0.137%
40	14.327	2077	2081	2084	rBV2	62439	78540	2.28%	0.274%
41	14.374	2084	2089	2091	rBV2	39701	59662	1.73%	0.208%
42	14.451	2100	2102	2104	rBV2	60723	44143	1.28%	0.154%
43	14.474	2104	2106	2108	rBV2	41475	36739	1.07%	0.128%
44	14.574	2120	2123	2128	rBV3	123494	195860	5.69%	0.683%
45	14.621	2128	2131	2133	rVV	99835	133125	3.87%	0.464%
46	14.674	2137	2140	2141	rVV2	83224	90067	2.62%	0.314%
47	14.704	2141	2145	2151	rVB	127750	257902	7.49%	0.899%
48	14.757	2151	2154	2158	rBV3	65045	76157	2.21%	0.266%
49	14.868	2171	2173	2176	rVB2	48742	41786	1.21%	0.146%
50	14.980	2188	2192	2195	rBV	310547	443904	12.90%	1.548%
51	15.057	2202	2205	2208	rBV2	59132	56316	1.64%	0.196%
52	15.086	2208	2210	2214	rVB2	44764	48427	1.41%	0.169%
53	15.151	2215	2221	2222	rBV5	45071	81580	2.37%	0.285%
54	15.280	2239	2243	2249	rVB	206208	243055	7.06%	0.848%
55	15.339	2249	2253	2259	rBV	212341	279034	8.11%	0.973%
56	15.404	2259	2264	2268	rBV	637697	822122	23.88%	2.867%
57	15.639	2301	2304	2309	rVB2	49474	66784	1.94%	0.233%
58	15.874	2340	2344	2349	rVB2	64004	94448	2.74%	0.329%
59	16.686	2477	2482	2492	rVB6	43678	94467	2.74%	0.329%
60	16.874	2509	2514	2523	rVB3	95604	190090	5.52%	0.663%
61	17.321	2585	2590	2599	rVB2	62264	130852	3.80%	0.456%

Sum of corrected areas: 28674149

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Misc :
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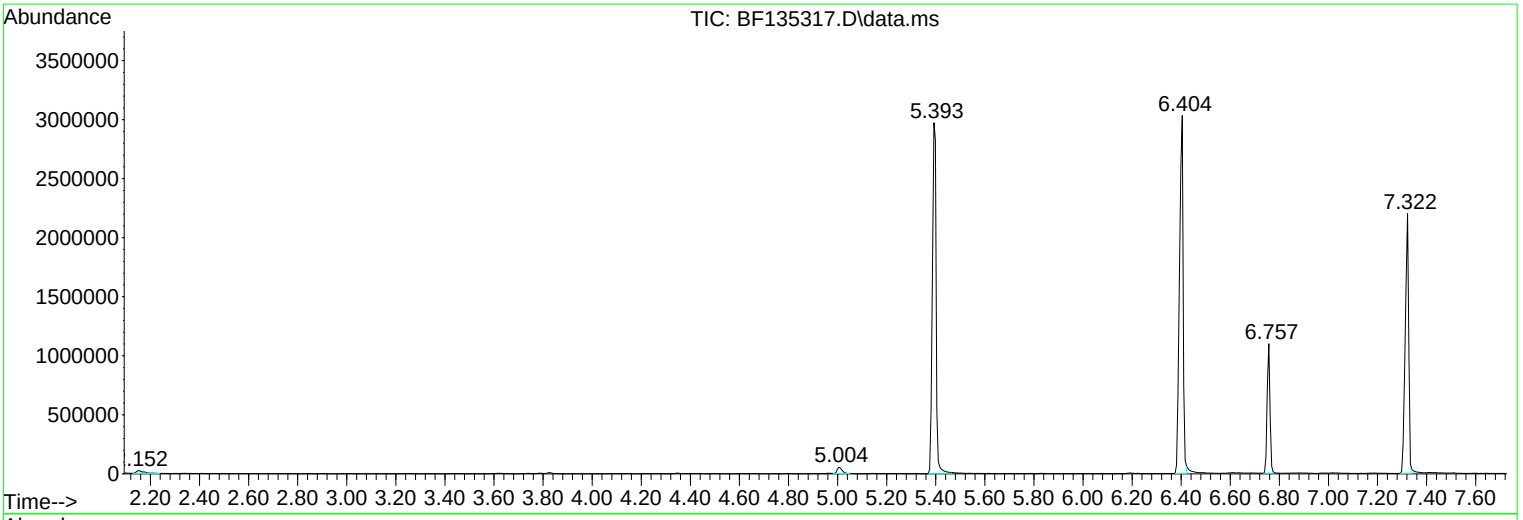
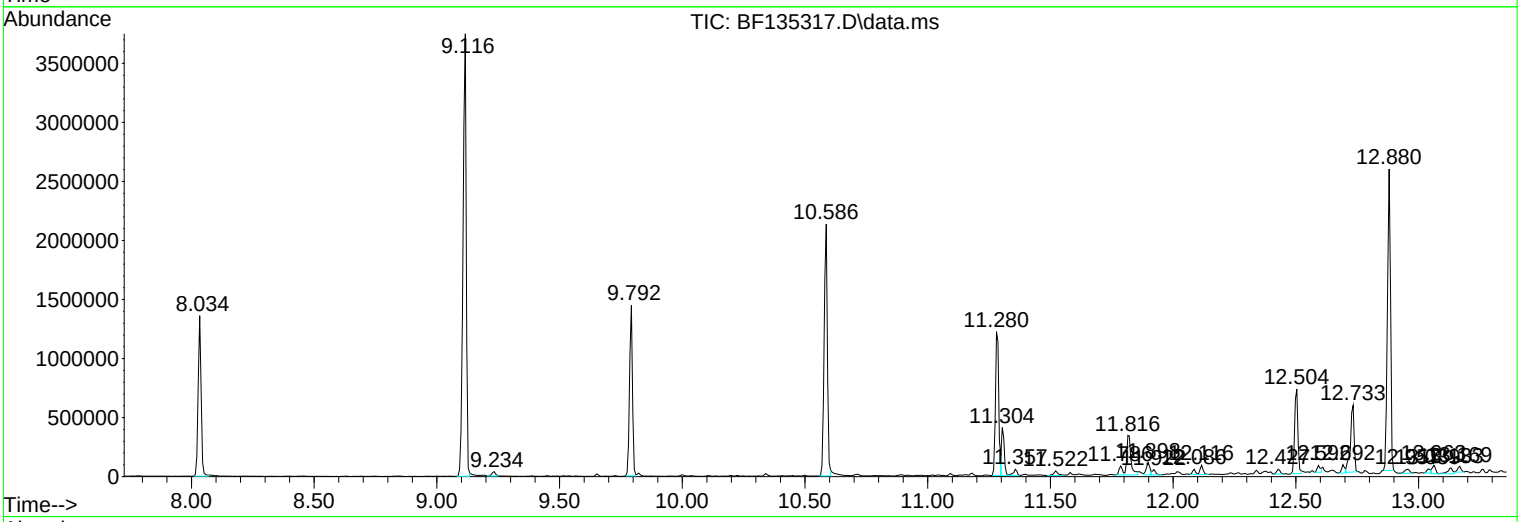
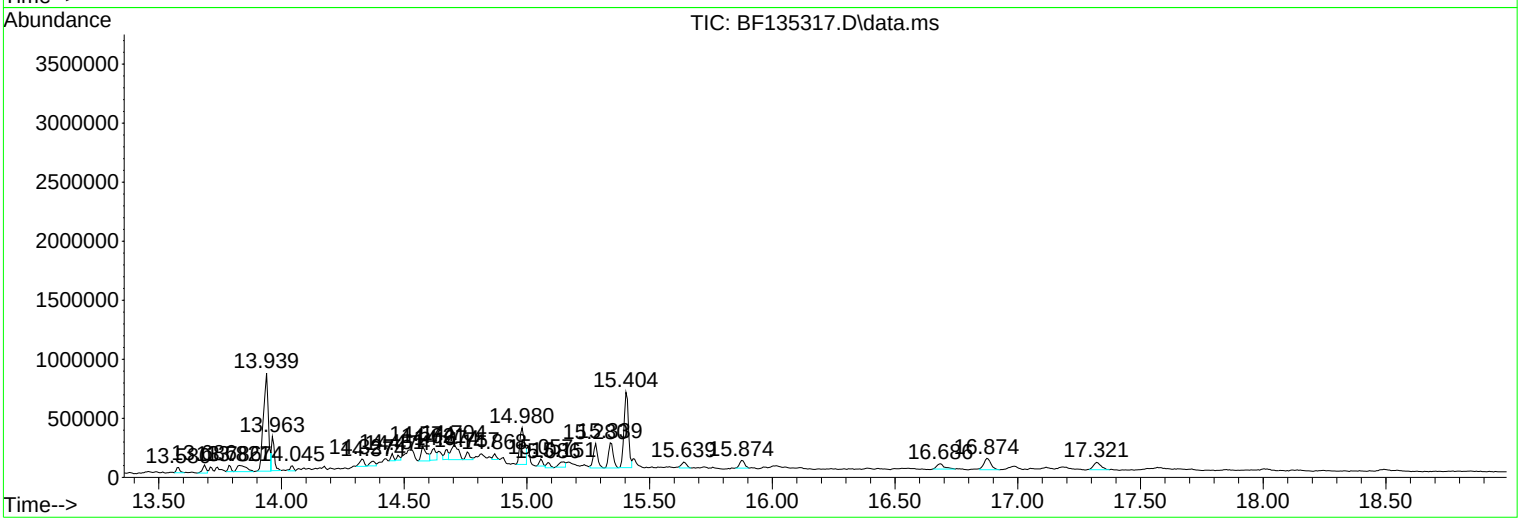
Instrument :
BNA_F
ClientSampleId :
72-11985

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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\BF091823\
Data File : BF135317.D
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Operator : CG\JU
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TIC Library : C:\Database\NIST20.L
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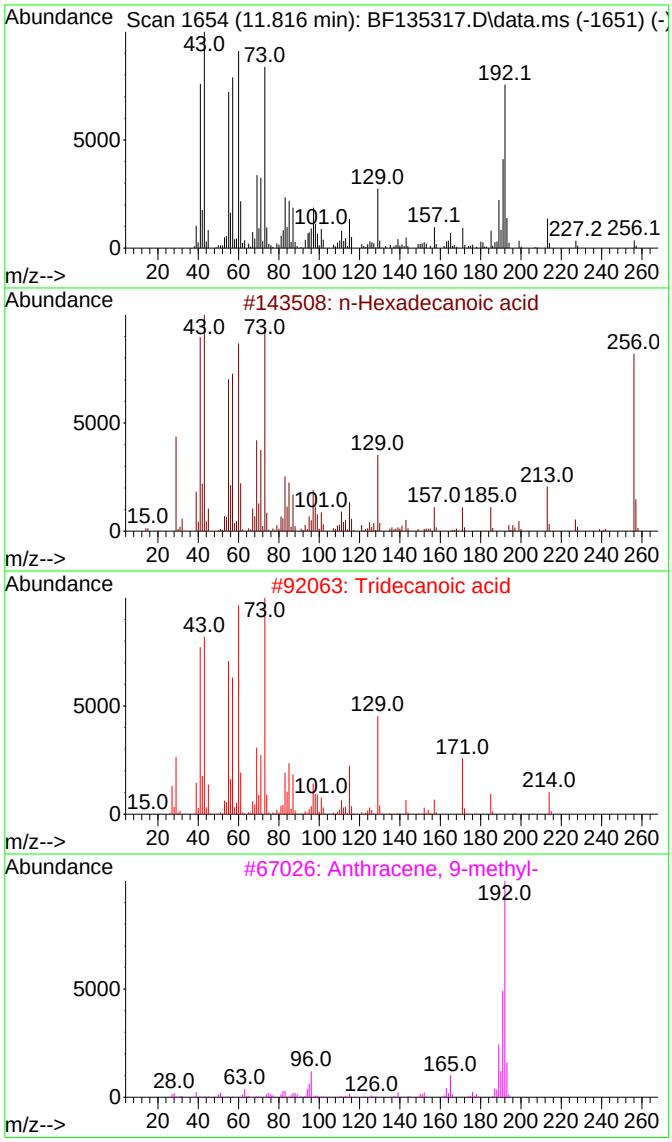
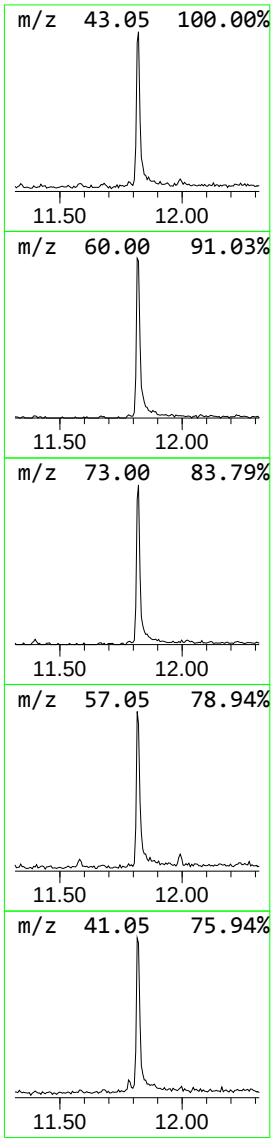
****

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.816	6.57 ng	383941	Phenanthrene-d10	11.281

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	86
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	86
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	80





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Misc :
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Instrument :
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ClientSampleId :
72-11985

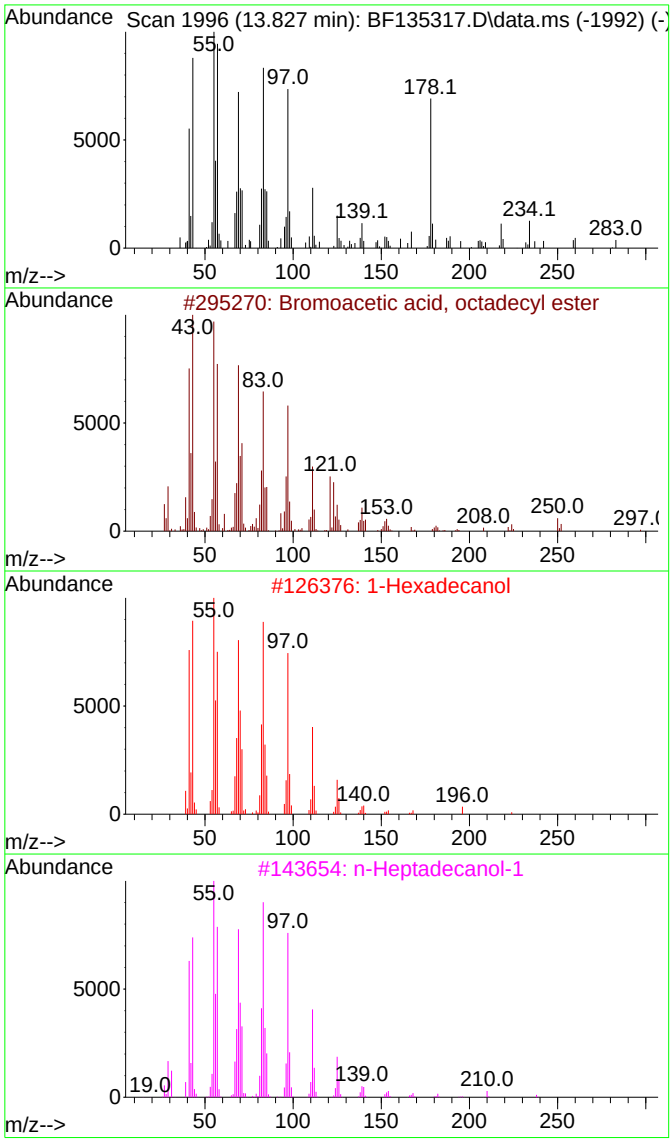
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

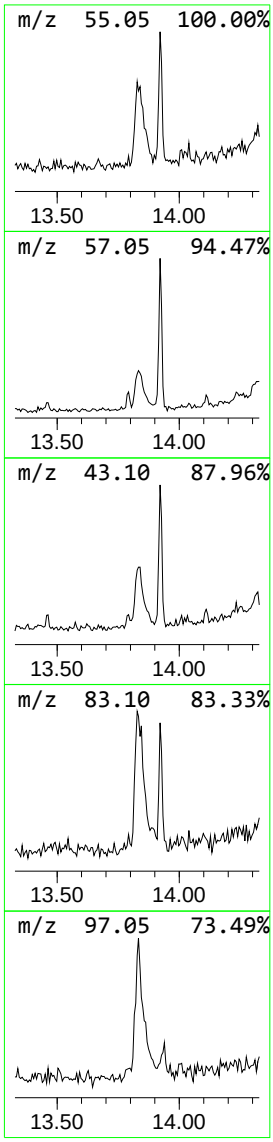
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Bromoacetic acid, octadecyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	2.43 ng	144248	Chrysene-d12	13.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	68
2	1-Hexadecanol	242	C16H34O	036653-82-4	68
3	n-Heptadecanol-1	256	C17H36O	001454-85-9	64
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	58
5	Carbonic acid, hexadecyl 2,2,2-t...	416	C19H35Cl3O3	1000314-56-2	52





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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

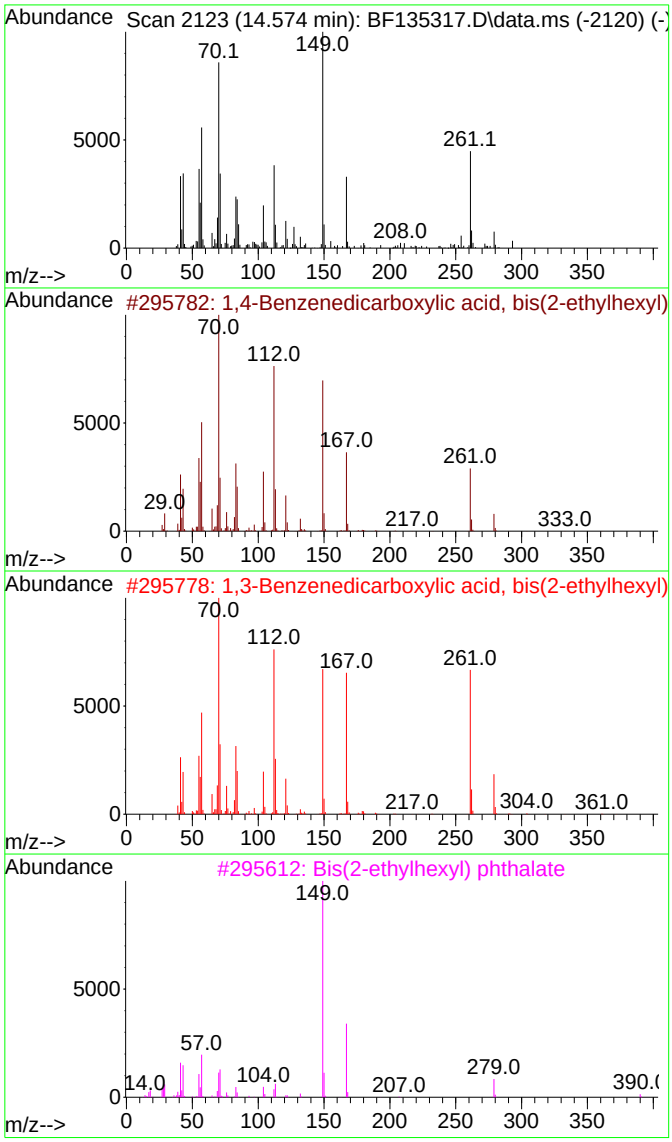
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

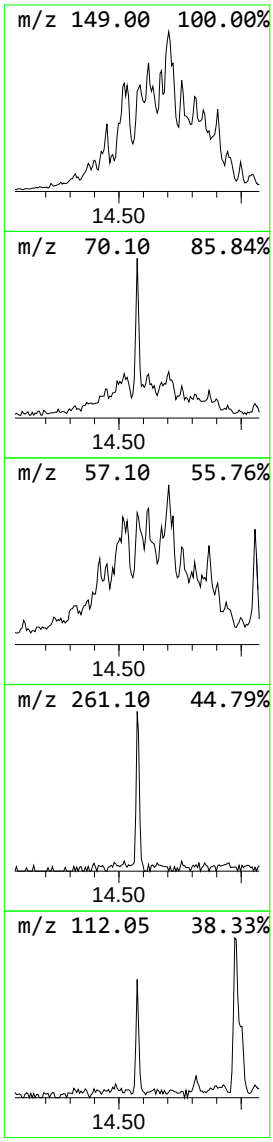
****

Peak Number 3 unknown14.574 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.574	3.30 ng	195860	Chrysene-d12	13.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	38
2	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	38
3	Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	27
4	Phthalic acid, di(oct-3-yl) ester	390	C24H38O4	1000377-72-3	27
5	Phthalic acid, octyl 4-isopropyl...	396	C25H32O4	1000315-22-4	27





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
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TIC Library : C:\Database\NIST20.L
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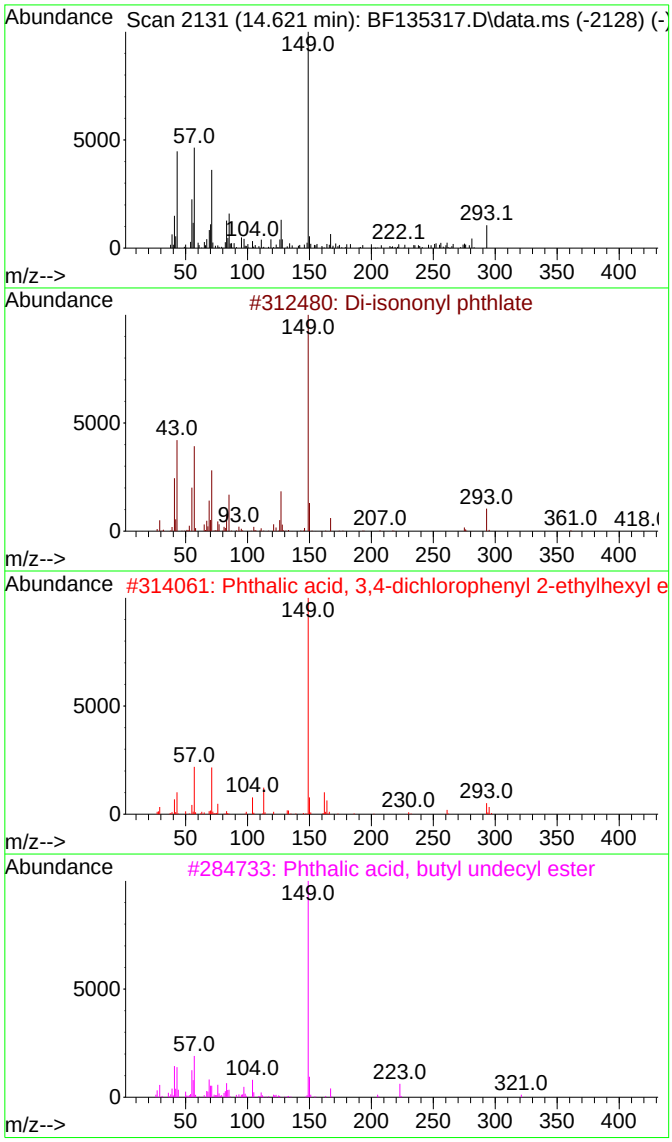
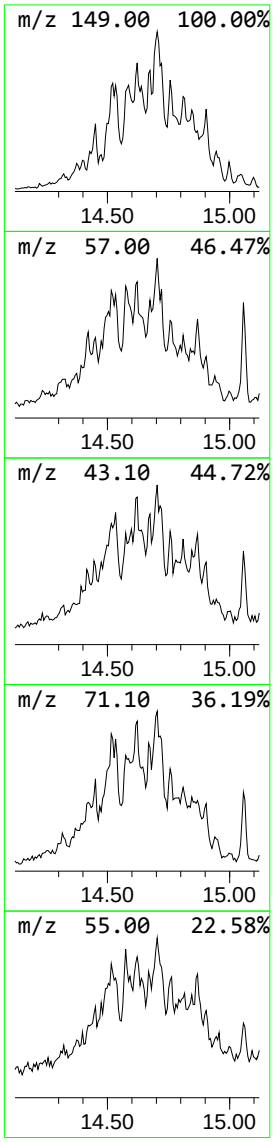
****

Peak Number 4 Di-isononyl phthlate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.621	2.24 ng	133125	Chrysene-d12	13.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-isononyl phthlate	418	C26H42O4	020548-62-3	64
2	Phthalic acid, 3,4-dichloropheny...	422	C22H24Cl2O4	1000315-52-0	59
3	Phthalic acid, butyl undecyl ester	376	C23H36O4	1000308-91-2	47
4	Phthalic acid, decyl pent-4-enyl...	374	C23H34O4	1000360-46-9	43
5	Diisooctyl phthalate	390	C24H38O4	000131-20-4	42





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Data File : BF135317.D
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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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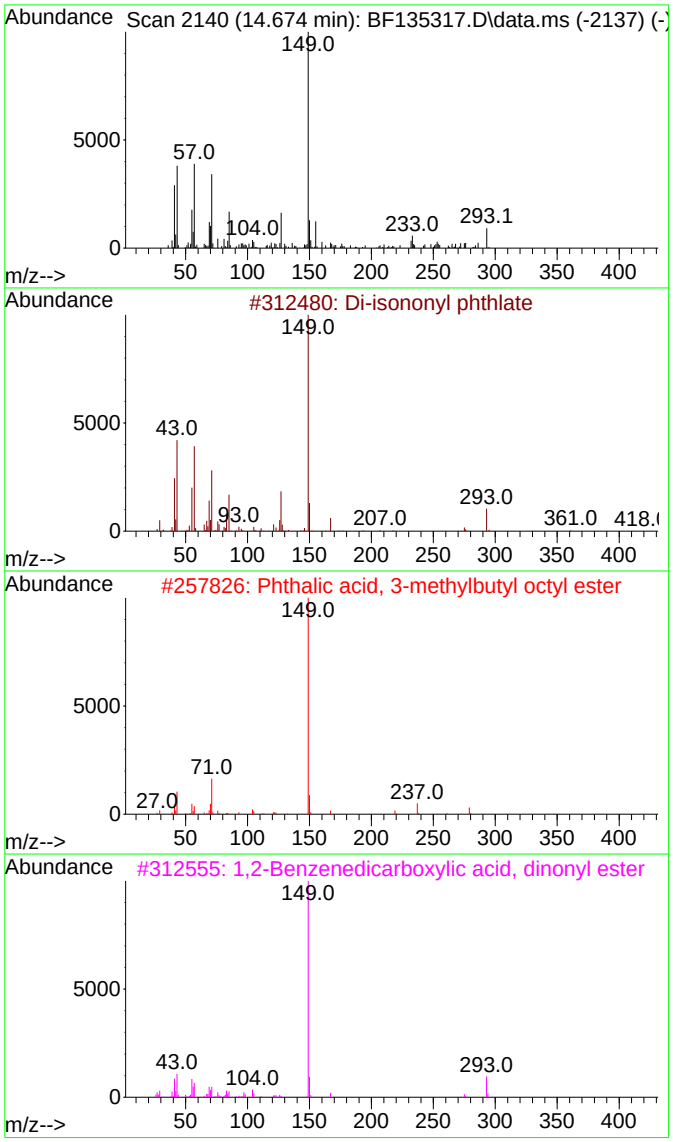
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

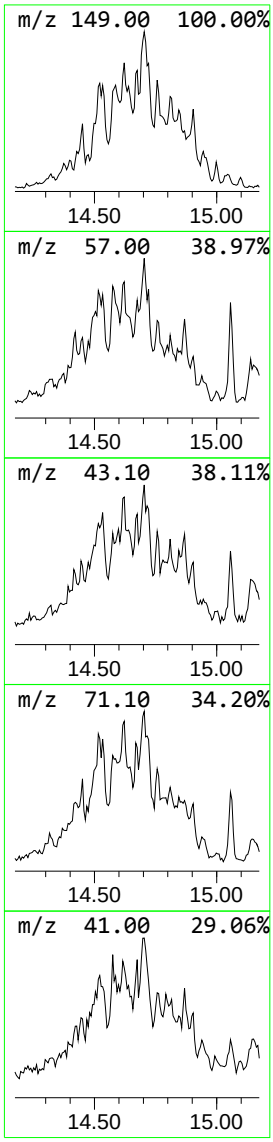
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Phthalic acid, 3-methylbuty... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.674	2.19 ng	90067	Perylene-d12	15.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-isononyl phthlate	418	C26H42O4	020548-62-3	80
2	Phthalic acid, 3-methylbutyl oct...	348	C21H32O4	1000356-80-9	50
3	1,2-Benzenedicarboxylic acid, di...	418	C26H42O4	000084-76-4	50
4	Phthalic acid, nonyl pentadecyl ...	502	C32H54O4	1000308-92-7	50
5	Phthalic acid, 5-methylhex-2-yl ...	502	C32H54O4	1000371-07-7	47





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Instrument :
BNA_F
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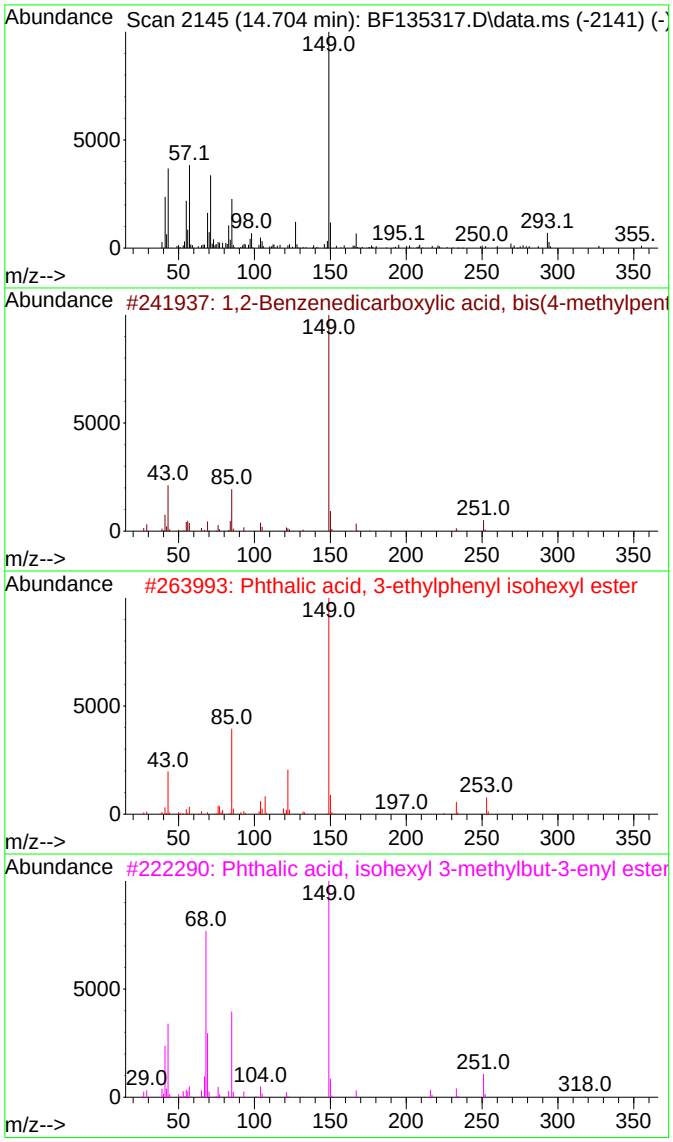
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

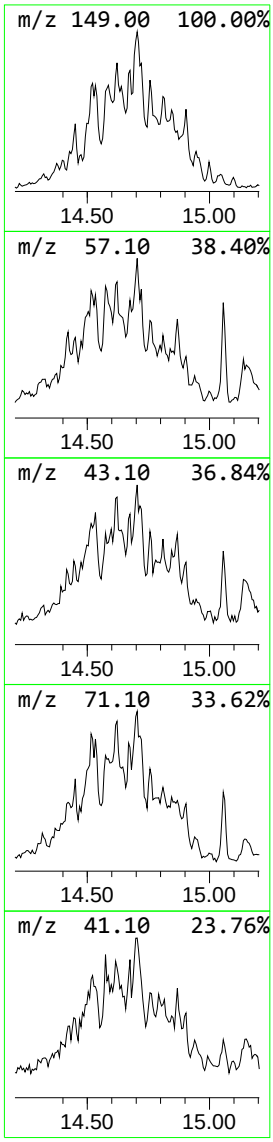
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1,2-Benzenedicarboxylic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.704	6.27 ng	257902	Perylene-d12	15.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenedicarboxylic acid, bi...	334	C20H30O4	000146-50-9	58
2	Phthalic acid, 3-ethylphenyl iso...	354	C22H26O4	1000357-08-0	53
3	Phthalic acid, isohexyl 3-methyl...	318	C19H26O4	1000357-10-3	53
4	Phthalic acid, hexyl 4-methylpen...	334	C20H30O4	1000356-87-6	53
5	Phthalic acid, 3-methylbut-3-eny...	360	C22H32O4	1010357-10-7	50





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Data File : BF135317.D
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Operator : CG\JU
Sample : 04399-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11985

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

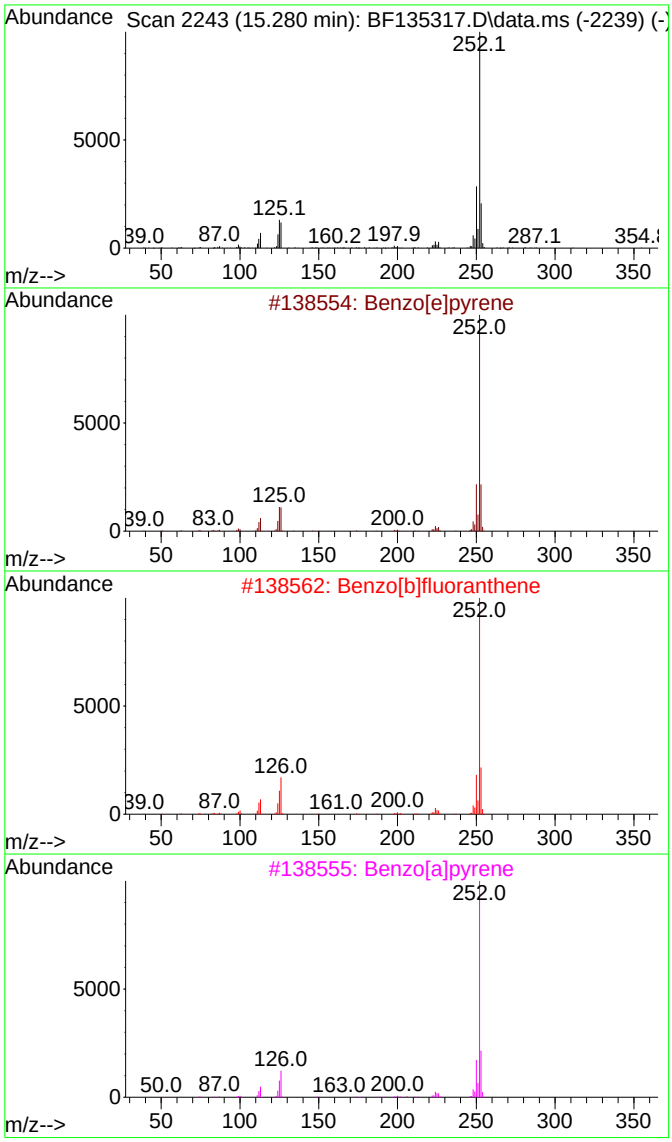
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

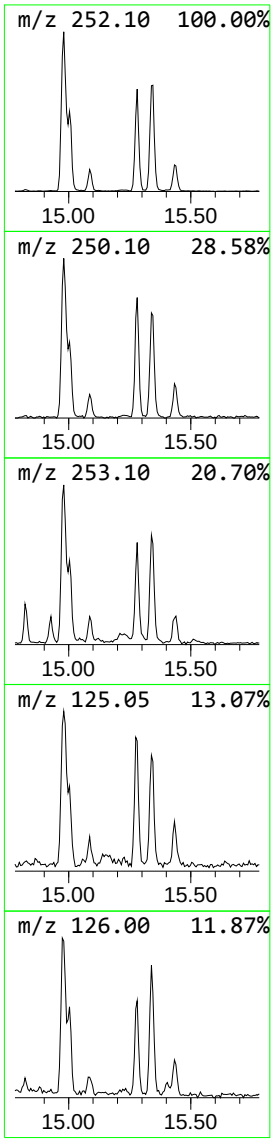
****

Peak Number 7 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.280	5.91 ng	243055	Perylene-d12	15.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	99
2	Benzo[b]fluoranthene	252	C20H12	000205-99-2	98
3	Benzo[a]pyrene	252	C20H12	000050-32-8	96
4	Perylene	252	C20H12	000198-55-0	96
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93





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Acq On : 18 Sep 2023 20:48
Operator : CG\JU
Sample : 04399-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11985

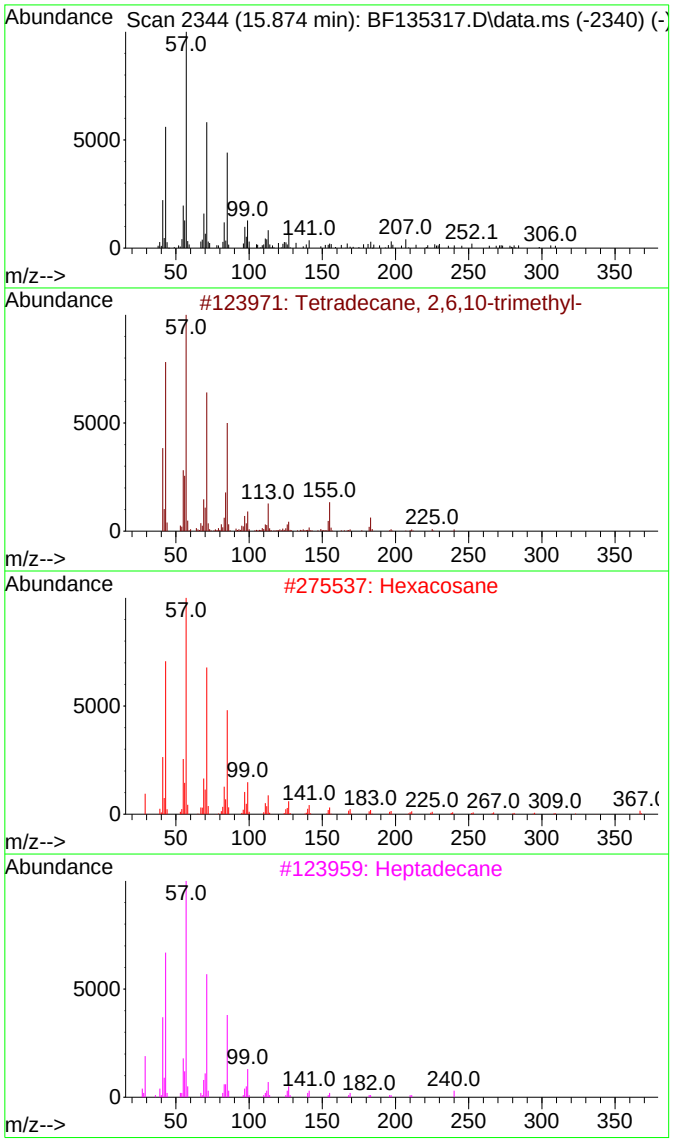
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

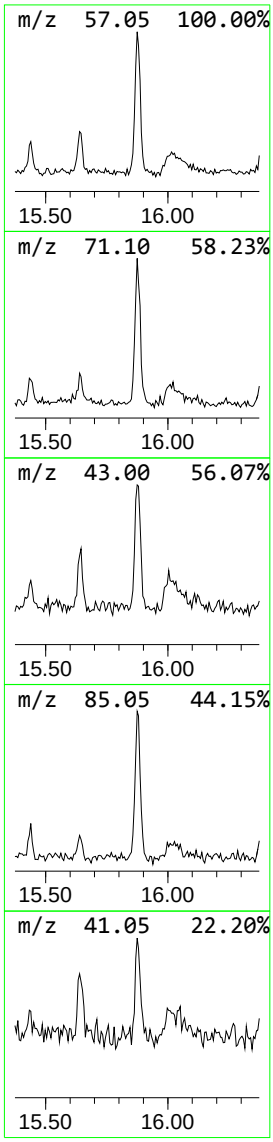
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Tetradecane, 2,6,10-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.874	2.30 ng	94448	Perylene-d12	15.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	87
2	Hexacosane	366	C26H54	000630-01-3	87
3	Heptadecane	240	C17H36	000629-78-7	87
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86
5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091823\
Data File : BF135317.D
Acq On : 18 Sep 2023 20:48
Operator : CG\JU
Sample : 04399-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11985

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

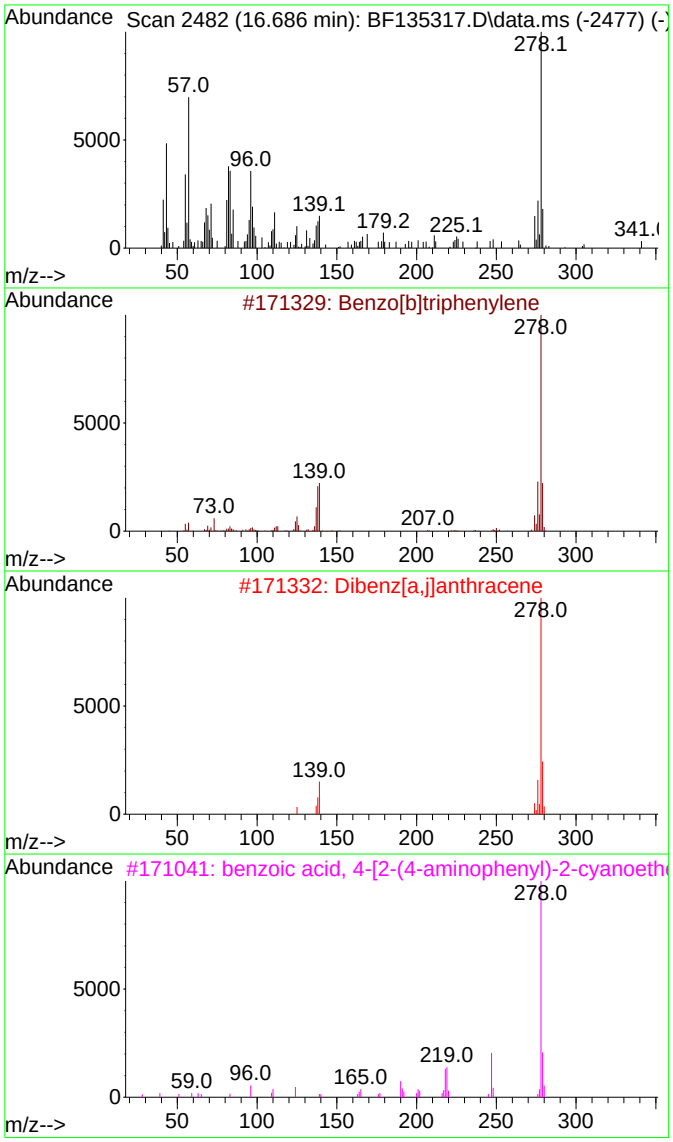
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

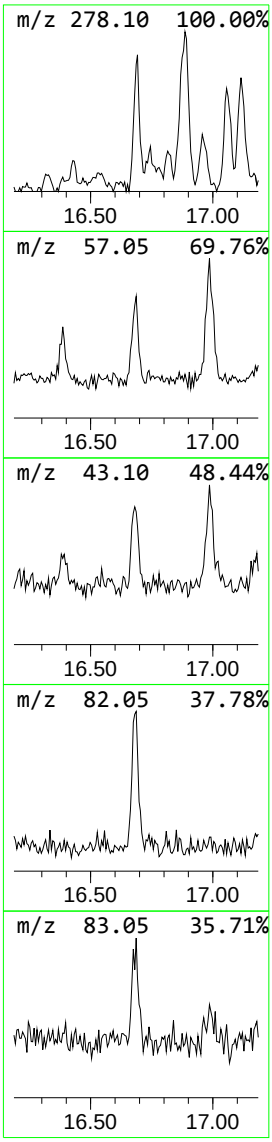
****

Peak Number 9 Benzo[b]triphenylene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.686	2.30 ng	94467	Perylene-d12	15.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]triphenylene	278	C22H14	000215-58-7	60
2	Dibenz[a,j]anthracene	278	C22H14	000224-41-9	53
3	benzoic acid, 4-[2-(4-aminopheny...	278	C17H14N2O2	1000397-13-0	49
4	O-Methylmurrayamine A	293	C19H19NO2	134779-20-7	47
5	Vanadium, (.eta.5-2,4-cyclopenta...	278	C17H23V	126948-97-8	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091823\
Data File : BF135317.D
Acq On : 18 Sep 2023 20:48
Operator : CG\JU
Sample : 04399-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11985

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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
n-Hexadecanoic ...	11.816	6.6	ng	383941	4	11.281	1169340	20.0
Bromoacetic aci...	13.827	2.4	ng	144248	5	13.939	1187920	20.0
unknown14.574	14.574	3.3	ng	195860	5	13.939	1187920	20.0
Di-isononyl pht...	14.621	2.2	ng	133125	5	13.939	1187920	20.0
Phthalic acid, ...	14.674	2.2	ng	90067	6	15.404	822122	20.0
1,2-Benzenedica...	14.704	6.3	ng	257902	6	15.404	822122	20.0
Benzo[e]pyrene	15.280	5.9	ng	243055	6	15.404	822122	20.0
Tetradecane, 2,...	15.874	2.3	ng	94448	6	15.404	822122	20.0
Benzo[b]triphen...	16.686	2.3	ng	94467	6	15.404	822122	20.0