LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091523\
Data File : BF135289.D
Acq On : 15 Sep 2023 20:26
Operator : CG\JU
Sample : 04399-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11930

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: BF135289.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.157	8	12	21	rVB2	31609	50351	1.60%	0.205%
2	5.010	492	497	507	rVB	58428	85858	2.73%	0.349%
3	5.398	558	563	566	rBV	2815441	2902663	92.36%	11.815%
4	6.404	728	734	737	rBV	2736307	2881284	91.68%	11.728%
5	6.592	764	766	774	rBV	35436	47194	1.50%	0.192%
6	6.757	790	794	798	rBV	849422	674732	21.47%	2.747%
7	7.322	885	890	893	rBV	1999414	1897502	60.37%	7.724%
8	8.033	1007	1011	1015	rBV	1011128	855102	27.21%	3.481%
9	9.116	1189	1195	1198	rBV	3473402	3142890	100.00%	12.793%
10	9.233	1211	1215	1219	rBV	43999	39916	1.27%	0.162%
11	9.792	1305	1310	1313	rBV	1087213	894089	28.45%	3.639%
12	10.586	1440	1445	1448	rBV	1909292	1690445	53.79%	6.881%
13	11.286	1560	1564	1566	rBV	873168	820139	26.10%	3.338%
14	11.304	1566	1567	1571	rVV	181766	145436	4.63%	0.592%
15	11.357	1572	1576	1580	rVB	31135	36518	1.16%	0.149%
16	11.821	1651	1655	1659	rBV	227906	209631	6.67%	0.853%
17	11.898	1665	1668	1671	rBV	39447	40893	1.30%	0.166%
18	12.504	1767	1771	1775	rBV	413146	348481	11.09%	1.419%
19	12.610	1784	1789	1793	rBV4	46331	62005	1.97%	0.252%
20	12.733	1805	1810	1813	rVB	333947	322316	10.26%	1.312%
21	12.886	1831	1836	1839	rVB	2355462	2254347	71.73%	9.176%
22	13.062	1864	1866	1870	rVB	39241	39440	1.25%	0.161%
23	13.133	1873	1878	1881	rBV2	28631	37984	1.21%	0.155%
24	13.686	1967	1972	1975	rBV	45996	52040	1.66%	0.212%
25	13.792	1987	1990	1991	rBV	36019	33473	1.07%	0.136%
26	13.821	1991	1995	2007	rVB5	55318	141615	4.51%	0.576%
27	13.939	2009	2015	2018	rBV2	741501	1144083	36.40%	4.657%
28	13.962	2018	2019	2023	rVB	145433	116262	3.70%	0.473%
29	14.327	2073	2081	2085	rBV5	70240	159320	5.07%	0.649%
30	14.374	2085	2089	2092	rBV3	37573	61398	1.95%	0.250%
31	14.427	2095	2098	2100	rBV3	38260	44499	1.42%	0.181%
32	14.451	2100	2102	2105	rBV2	77400	69176	2.20%	0.282%
33	14.521	2108	2114	2115	rBV	136745	188507	6.00%	0.767%
34	14.580	2120	2124	2128	rVV	477306	573380	18.24%	2.334%
35	14.621	2129	2131	2134	rVV	172628	242221	7.71%	0.986%
36	14.674	2138	2140	2142	rVV2	117149	138144	4.40%	0.562%

LSC Area Percent Report

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Misc :
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Instrument :
BNA_F
ClientSampleId :
72-11930

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

37	14.709	2142	2146	2152	rVB	186946	375003	11.93%	1.526%
38	14.762	2152	2155	2157	rBV	100310	93889	2.99%	0.382%
39	14.815	2162	2164	2168	rVB3	62554	68078	2.17%	0.277%
40	14.980	2189	2192	2195	rBV	155655	190948	6.08%	0.777%
41	15.062	2203	2206	2209	rVB2	43164	49485	1.57%	0.201%
42	15.139	2214	2219	2223	rBV8	23314	46409	1.48%	0.189%
43	15.280	2239	2243	2249	rVB	108023	141133	4.49%	0.574%
44	15.345	2249	2254	2259	rVV	124147	163071	5.19%	0.664%
45	15.409	2259	2265	2269	rVV	525887	682137	21.70%	2.777%
46	15.439	2269	2270	2278	rVB4	57215	61358	1.95%	0.250%
47	15.880	2341	2345	2353	rVB	51428	78725	2.50%	0.320%
48	16.874	2509	2514	2522	rVB2	53719	108658	3.46%	0.442%
49	17.321	2586	2590	2598	rVB	36379	64589	2.06%	0.263%

Sum of corrected areas: 24566817

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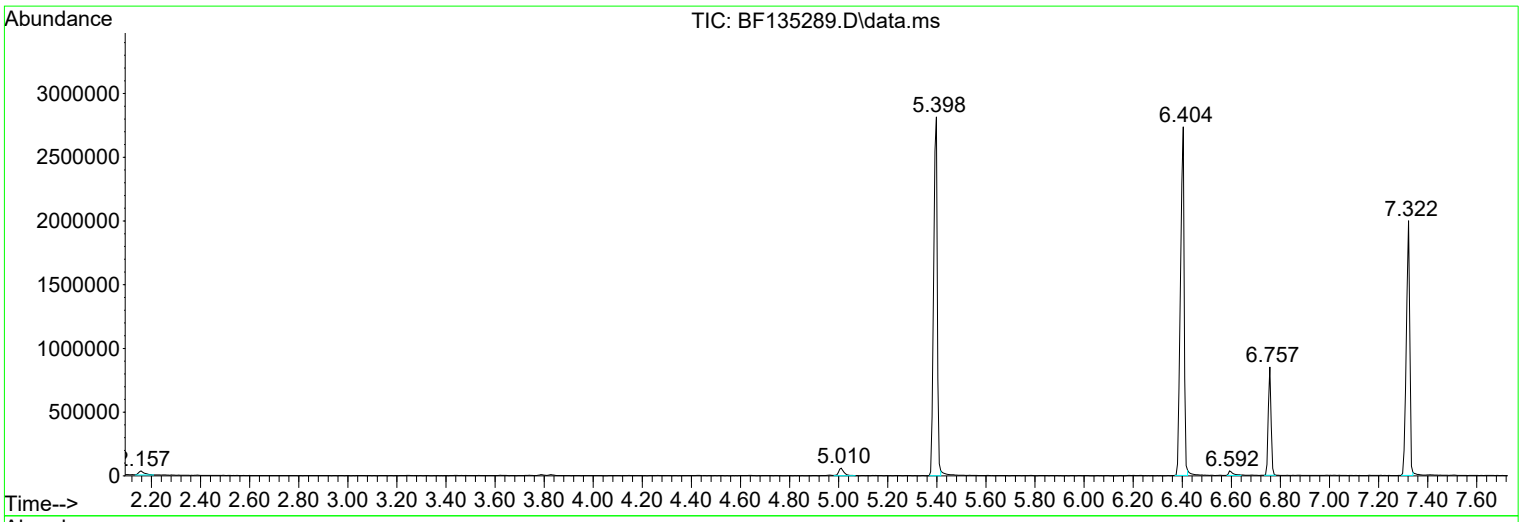
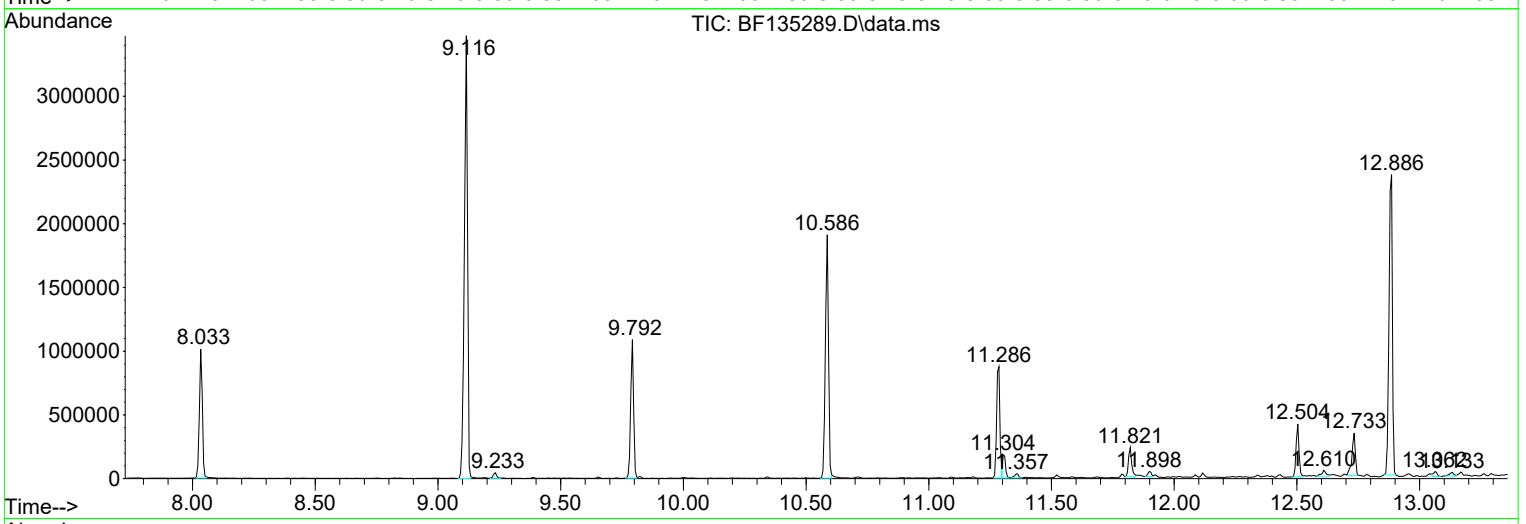
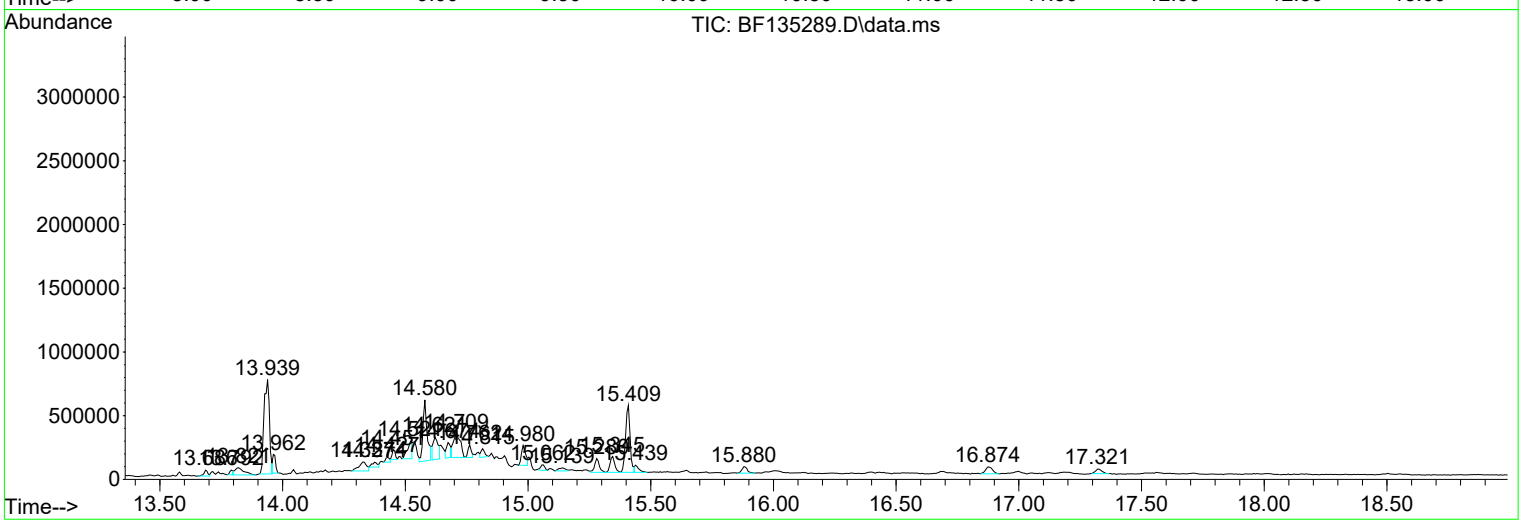
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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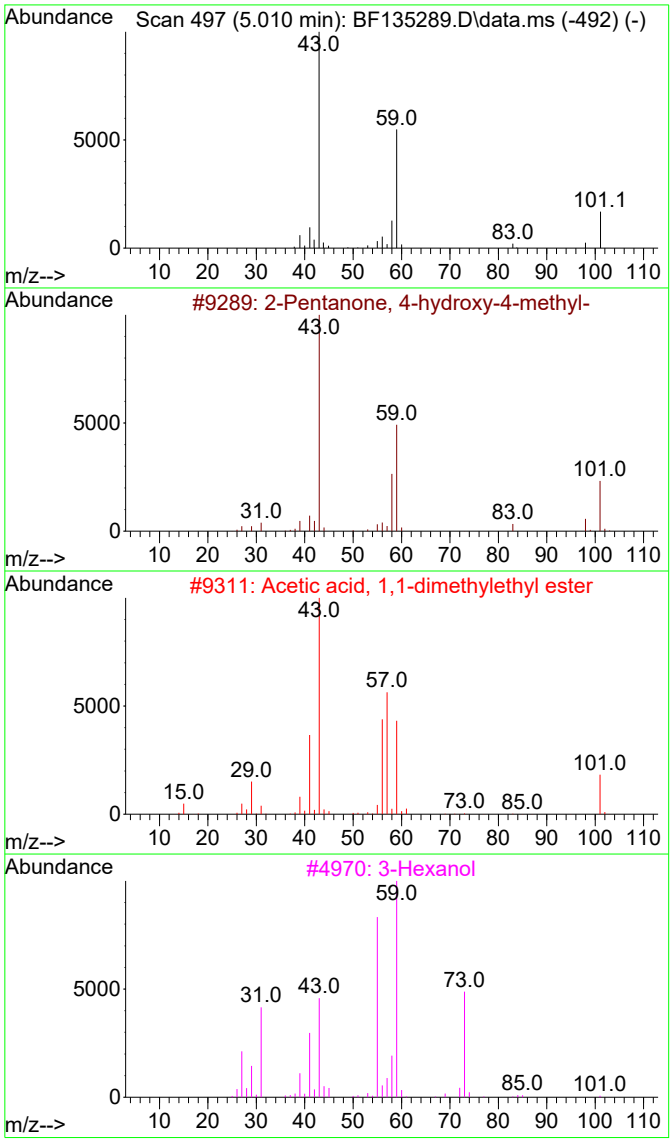
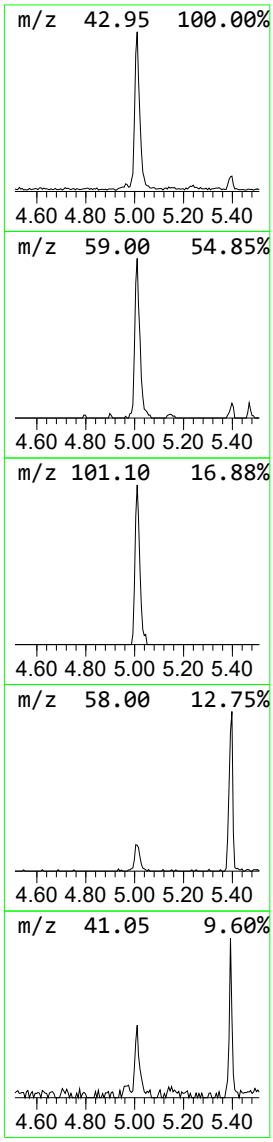
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.010	2.54 ng	85858	1,4-Dichlorobenzene-d4	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol	102	C6H14O	000623-37-0	33
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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

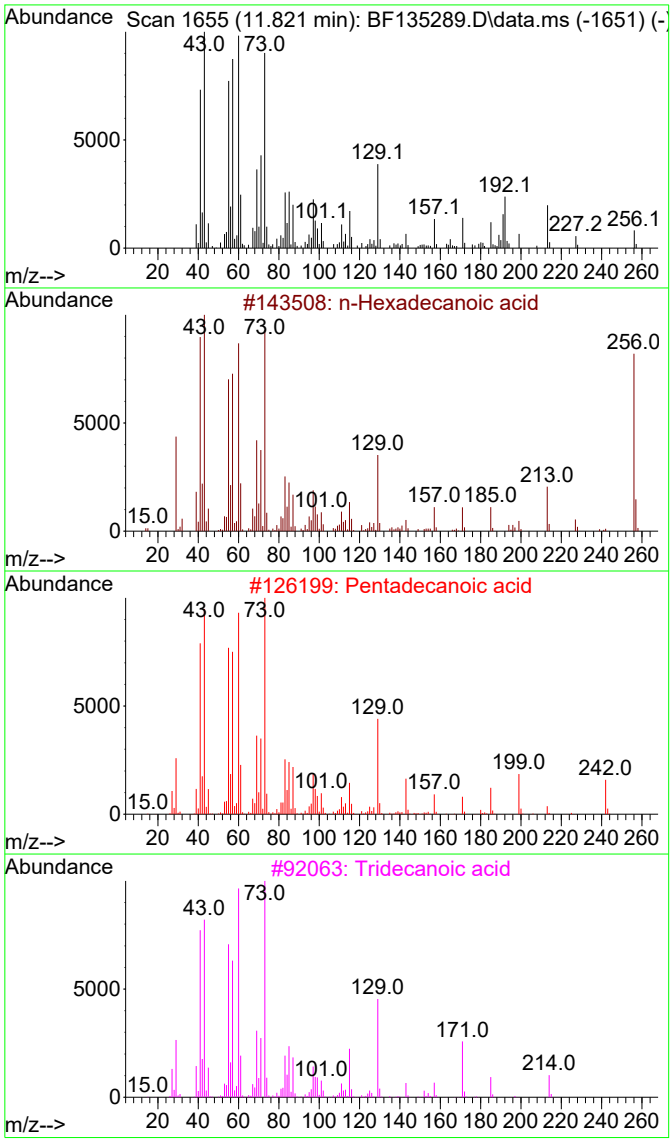
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

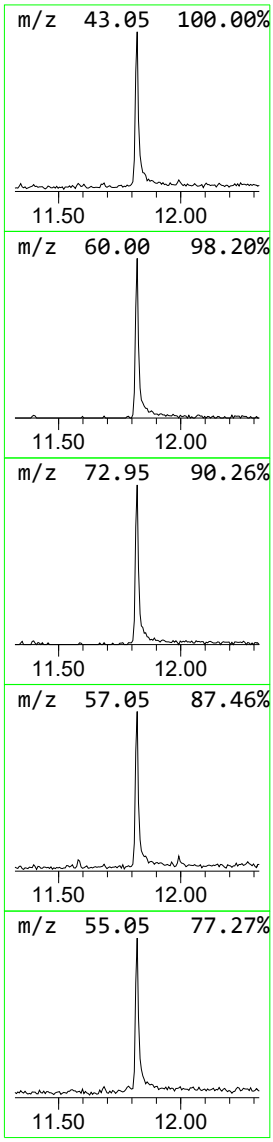
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.821	5.11 ng	209631	Phenanthrene-d10	11.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	86
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58





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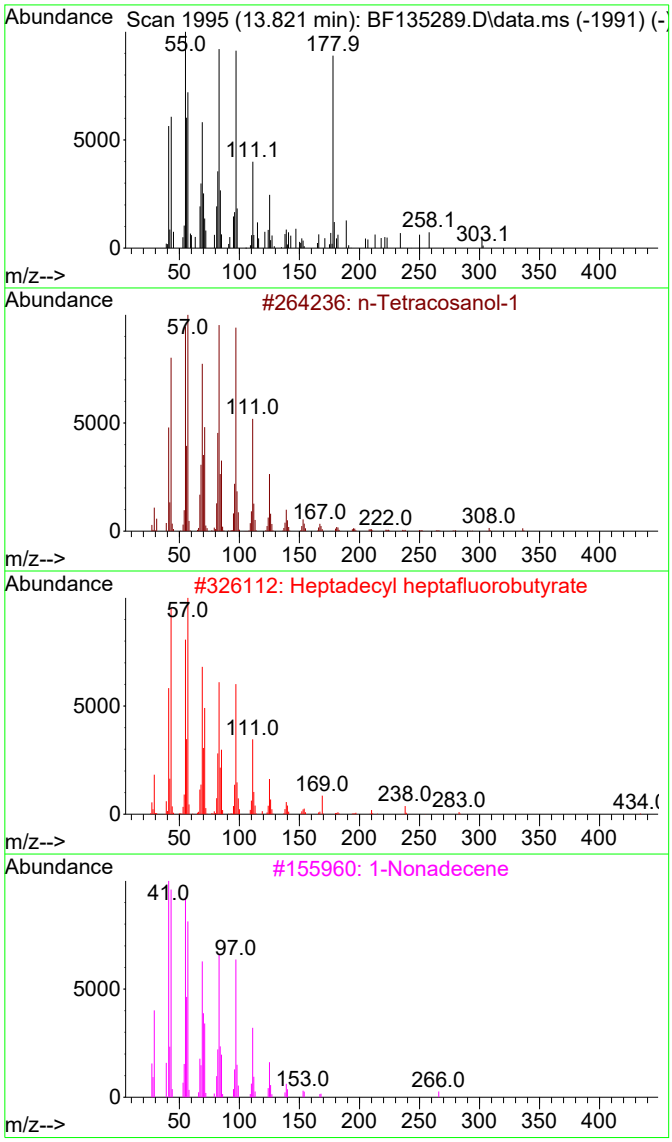
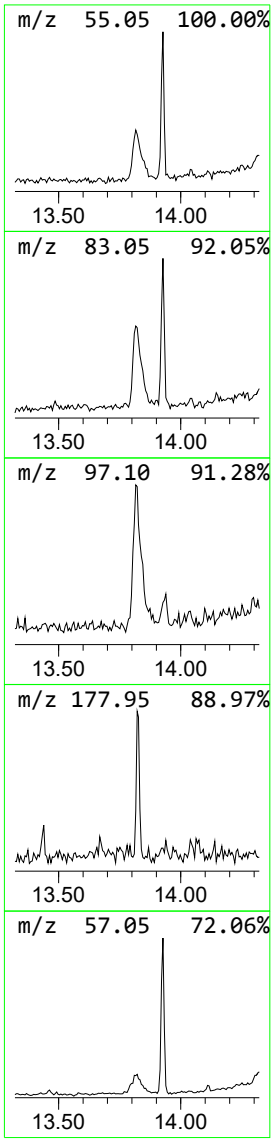
****

Peak Number 3 n-Tetracosanol-1 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.821	2.48 ng	141615	Chrysene-d12	13.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	70
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	64
3	1-Nonadecene	266	C19H38	018435-45-5	64
4	1-Octadecanol	270	C18H38O	000112-92-5	64
5	Behenic alcohol	326	C22H46O	000661-19-8	62





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ALS Vial : 14 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

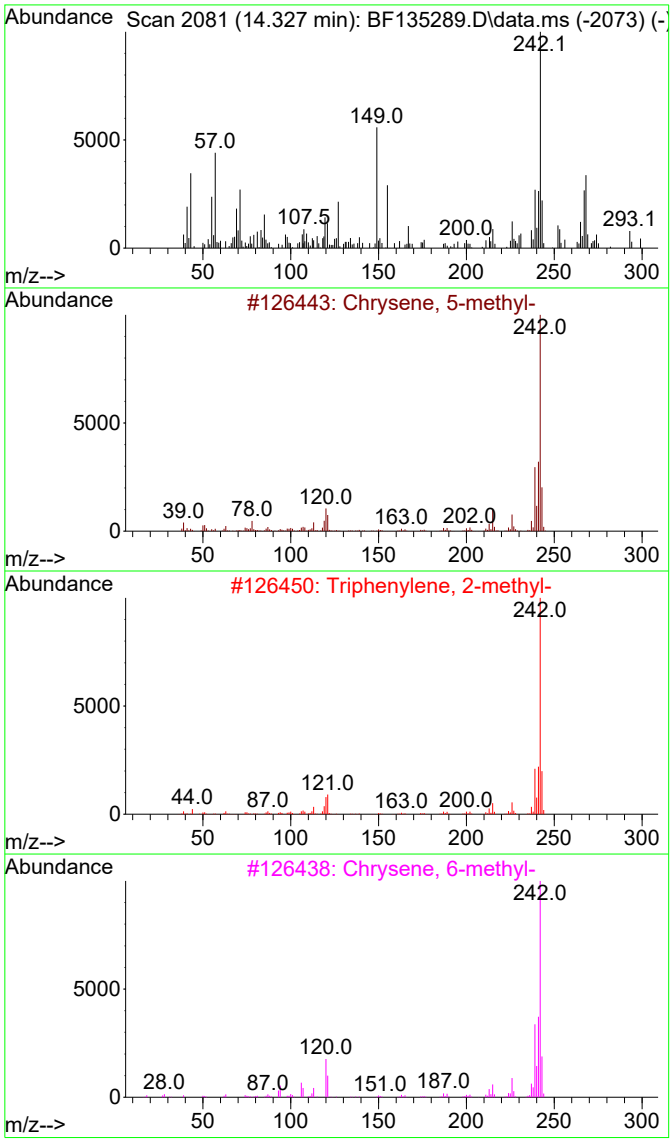
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

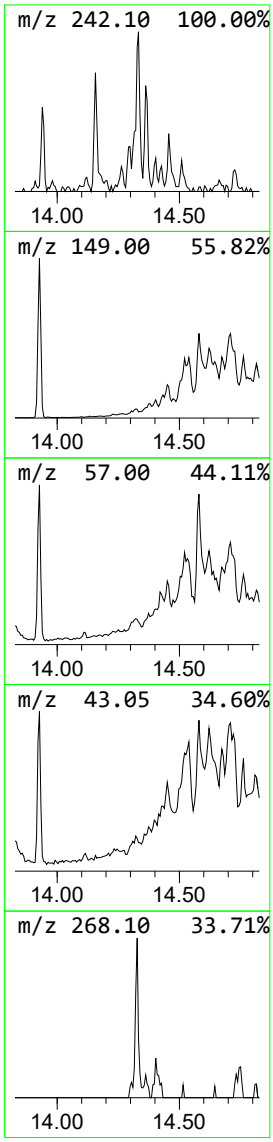
****

Peak Number 4 Chrysene, 5-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.327	2.79 ng	159320	Chrysene-d12	13.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Chrysene, 5-methyl-	242	C19H14	003697-24-3	86
2	Triphenylene, 2-methyl-	242	C19H14	001705-84-6	86
3	Chrysene, 6-methyl-	242	C19H14	001705-85-7	80
4	2-Methylchrysene	242	C19H14	003351-32-4	66
5	Benz[a]anthracene, 2-methyl-	242	C19H14	002498-76-2	64





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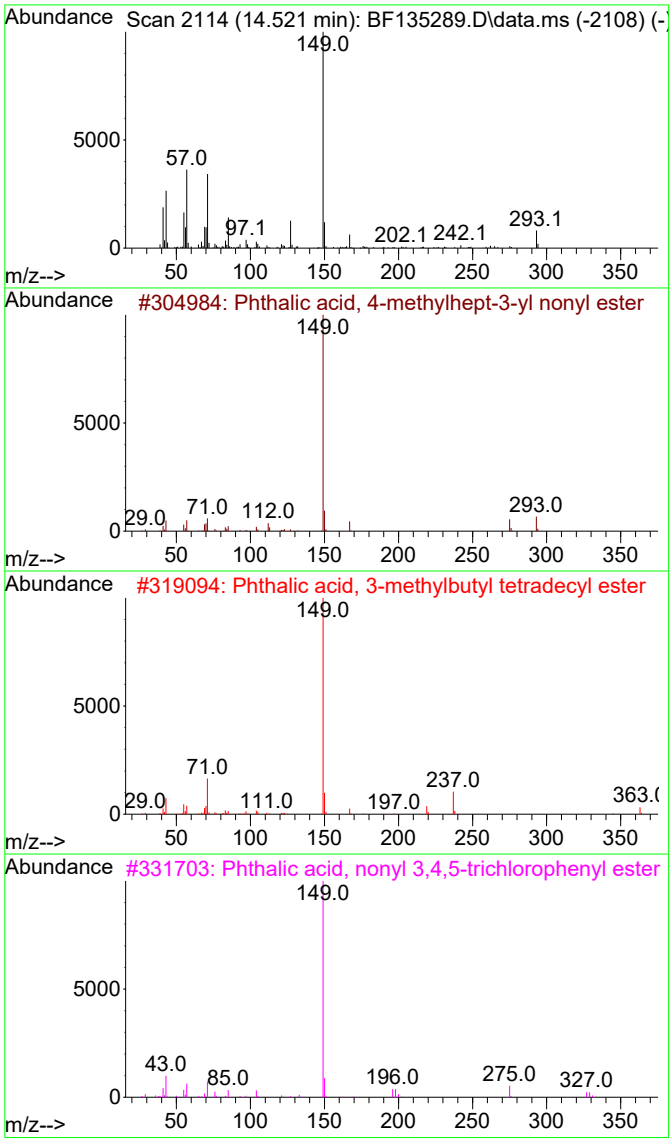
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

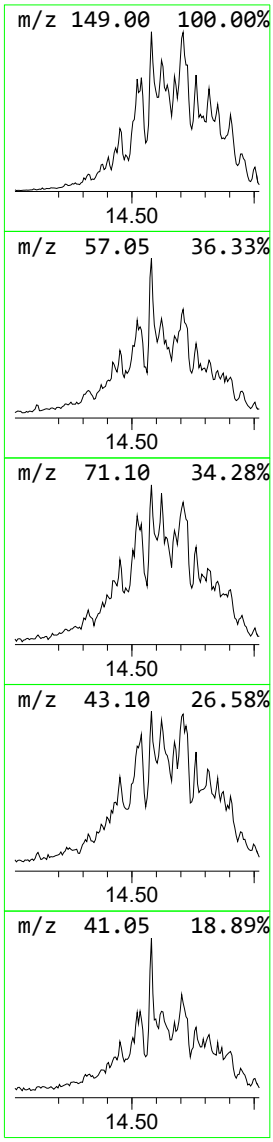
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Phthalic acid, 4-methylhept... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.521	3.30 ng	188507	Chrysene-d12	13.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic acid, 4-methylhept-3-yl...	404	C25H40O4	1000377-94-4	72
2	Phthalic acid, 3-methylbutyl tet...	432	C27H44O4	1000356-81-5	64
3	Phthalic acid, nonyl 3,4,5-trich...	470	C23H25Cl3O4	1010357-07-2	64
4	Phthalic acid, hexadecyl 3-methy...	460	C29H48O4	1000356-81-7	64
5	Phthalic acid, 3,4-dichloropheny...	422	C22H24Cl2O4	1000315-52-0	59





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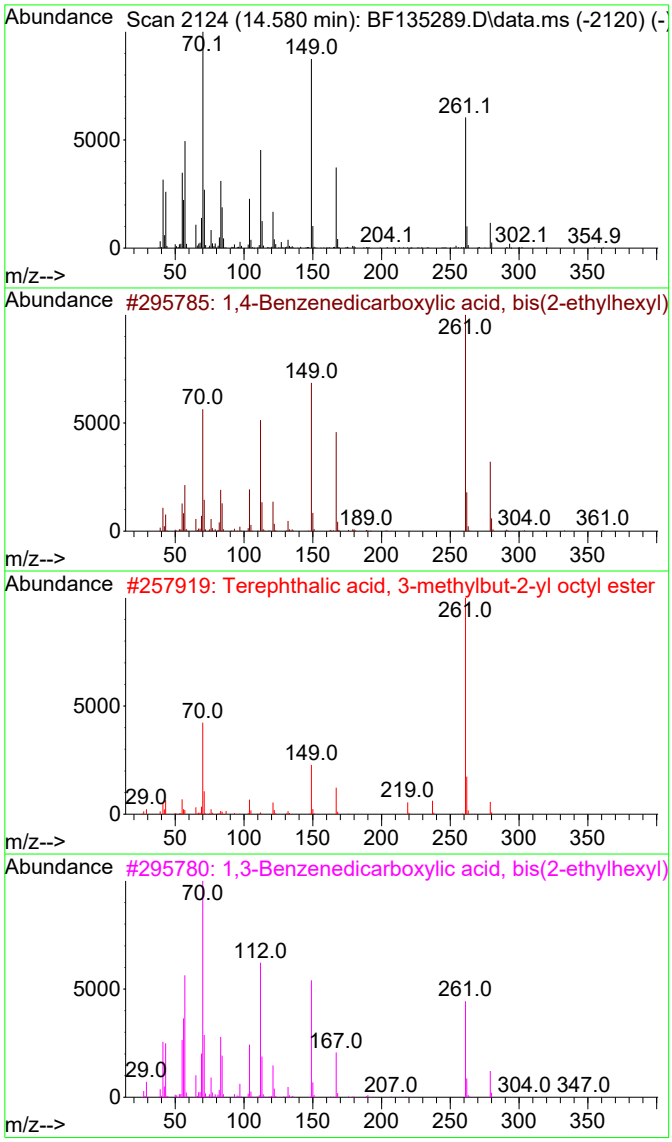
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

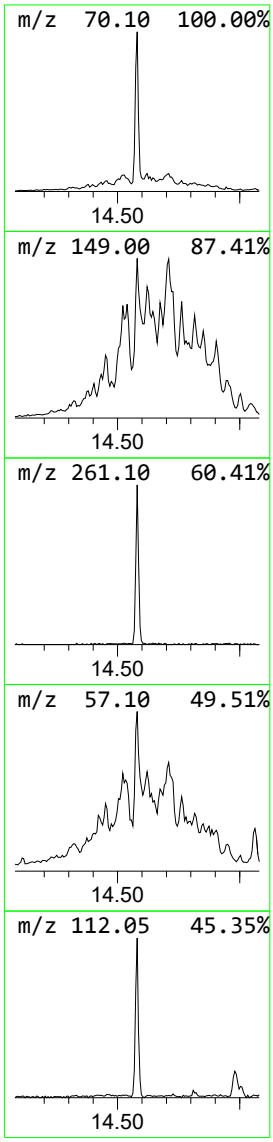
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1,4-Benzenedicarboxylic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.580	10.02 ng	573380	Chrysene-d12	13.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	76
2	Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	72
3	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	64
4	Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	35
5	Phthalic acid, but-3-yn-2-yl 3,5...	330	C18H12F2O4	1000315-75-6	35





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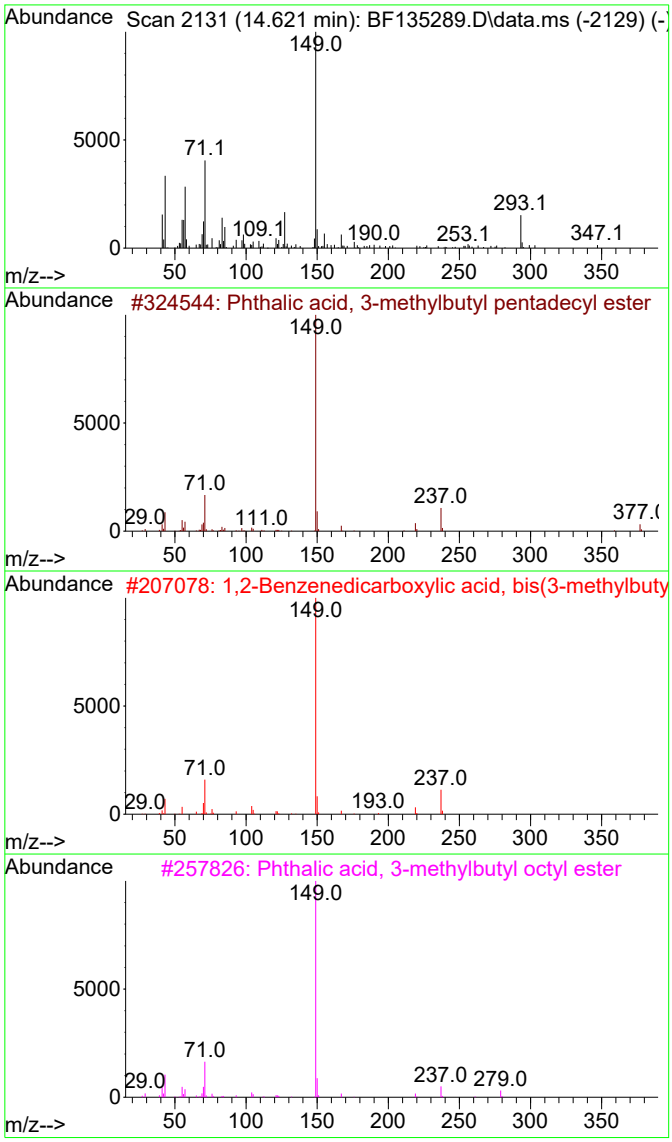
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

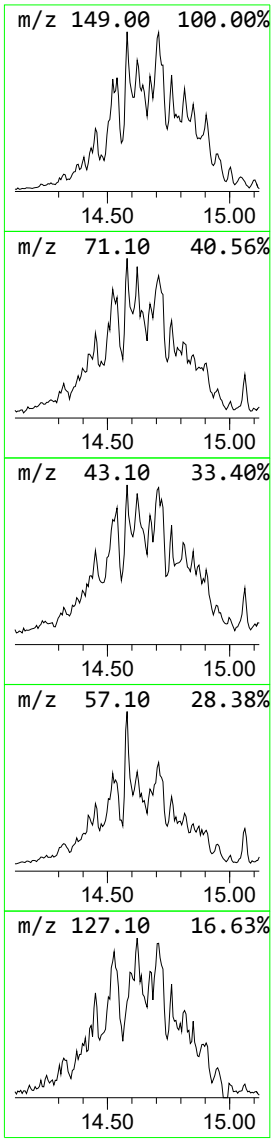
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Phthalic acid, 3-methylbuty... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.621	4.23 ng	242221	Chrysene-d12	13.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic acid, 3-methylbutyl pen...	446	C28H46O4	1000356-81-6	59
2	1,2-Benzenedicarboxylic acid, bi...	306	C18H26O4	000605-50-5	53
3	Phthalic acid, 3-methylbutyl oct...	348	C21H32O4	1000356-80-9	53
4	Phthalic acid, 3,4-dimethylpheny...	396	C25H32O4	1000309-82-3	47
5	Didecyl phthalate	446	C28H46O4	000084-77-5	43





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TIC Library : C:\Database\NIST20.L
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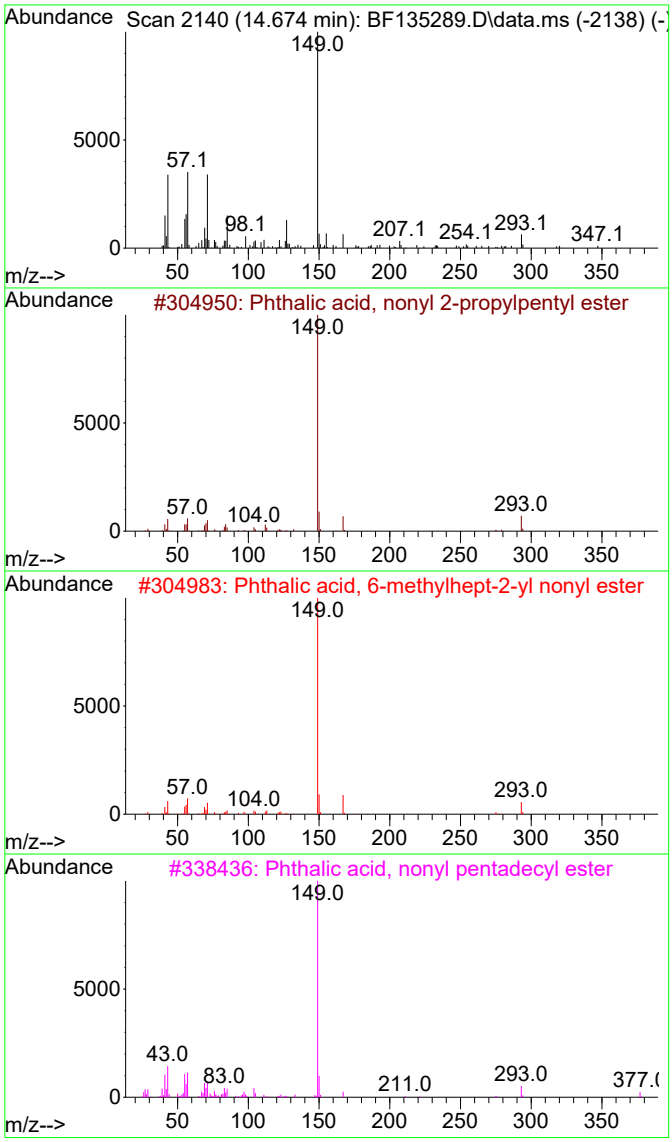
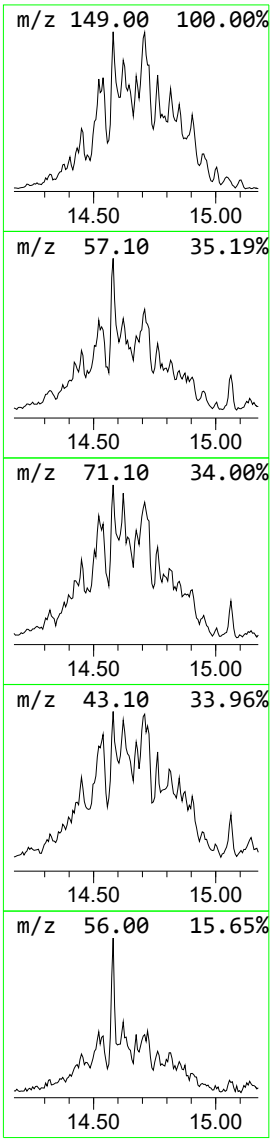
****
Peak Number 8 Phthalic acid, nonyl 2-prop... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.674	4.05 ng	138144	Perylene-d12	15.409

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic acid, nonyl 2-propylpen...	404	C25H40O4	1000377-92-5	53
2	Phthalic acid, 6-methylhept-2-yl...	404	C25H40O4	1000377-96-3	53
3	Phthalic acid, nonyl pentadecyl ...	502	C32H54O4	1000308-92-7	50
4	1,2-Benzenedicarboxylic acid, is...	418	C26H42O4	001330-96-7	47
5	Phthalic acid, 8-bromoctyl hexyl...	440	C22H33BrO4	1000382-55-6	47





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Data File : BF135289.D
Acq On : 15 Sep 2023 20:26
Operator : CG\JU
Sample : 04399-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11930

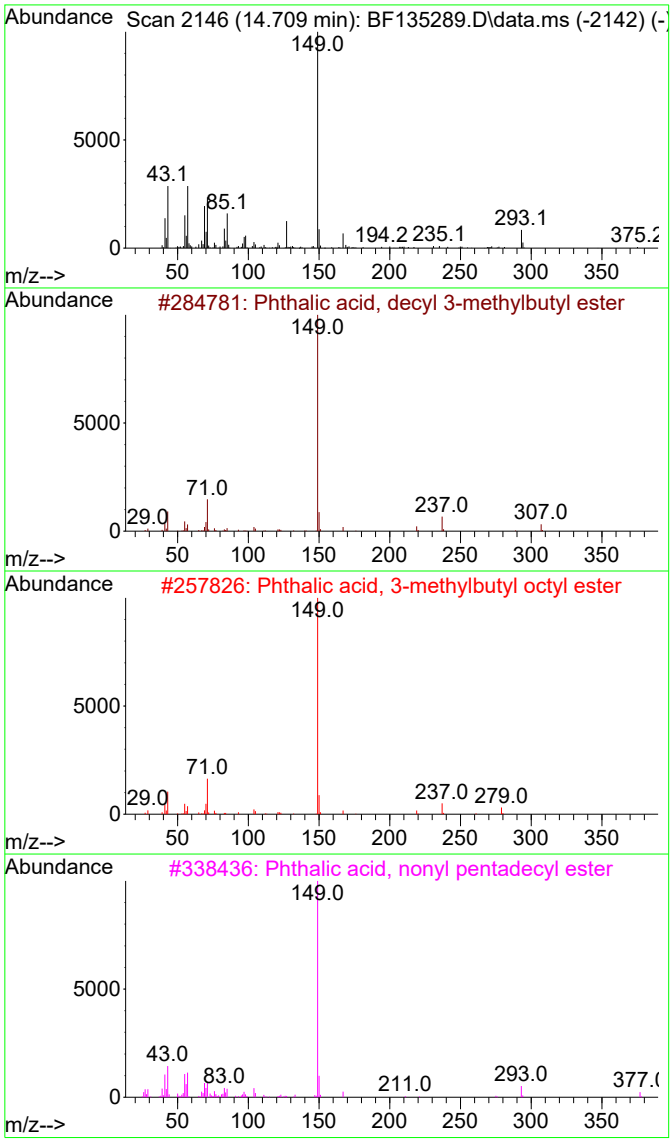
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

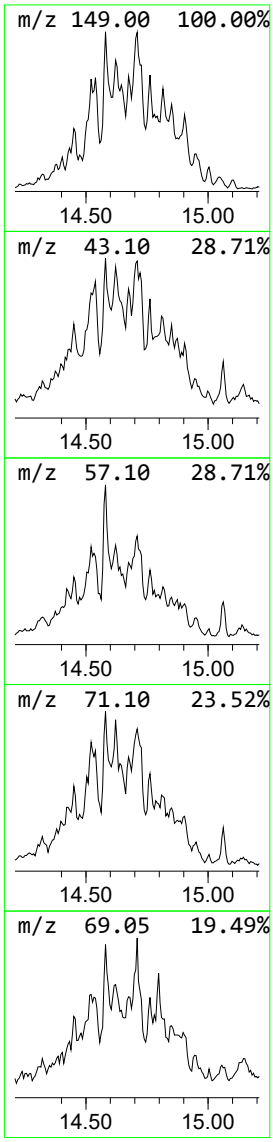
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Phthalic acid, decyl 3-meth... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.709	10.99 ng	375003	Perylene-d12	15.409

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic acid, decyl 3-methylbut...	376	C23H36O4	1000356-81-1	59
2	Phthalic acid, 3-methylbutyl oct...	348	C21H32O4	1000356-80-9	53
3	Phthalic acid, nonyl pentadecyl ...	502	C32H54O4	1000308-92-7	53
4	Phthalic acid, 2,4-dimethylpent-...	418	C26H42O4	1000356-85-0	53
5	Phthalic acid, 2,2-dimethylpent-...	446	C28H46O4	1000415-53-6	53





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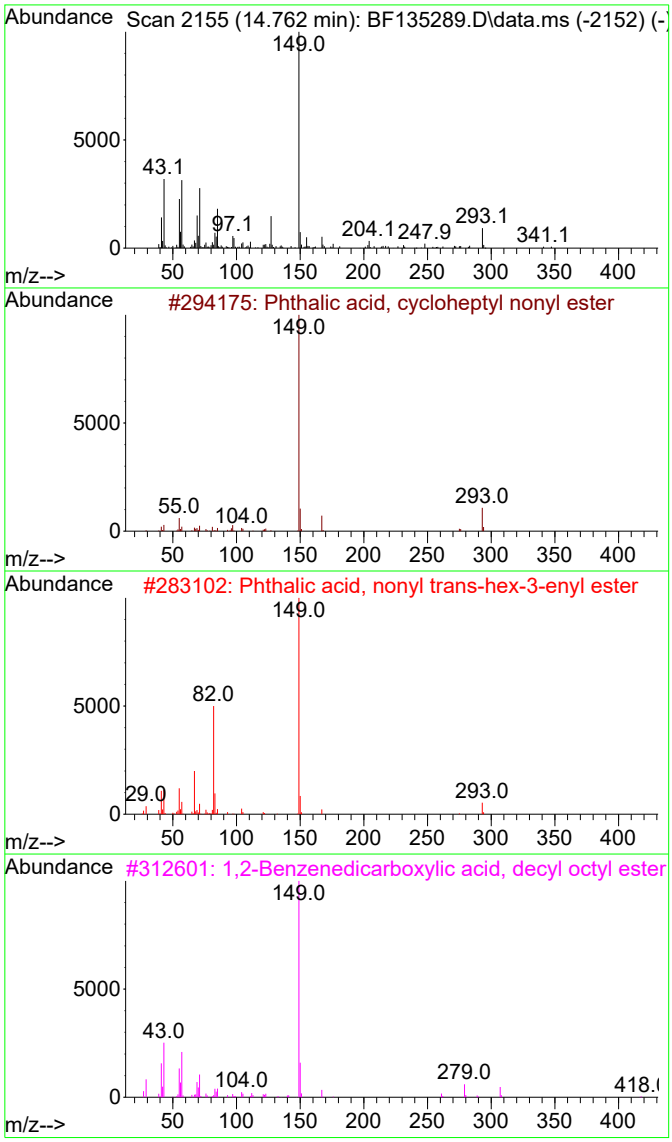
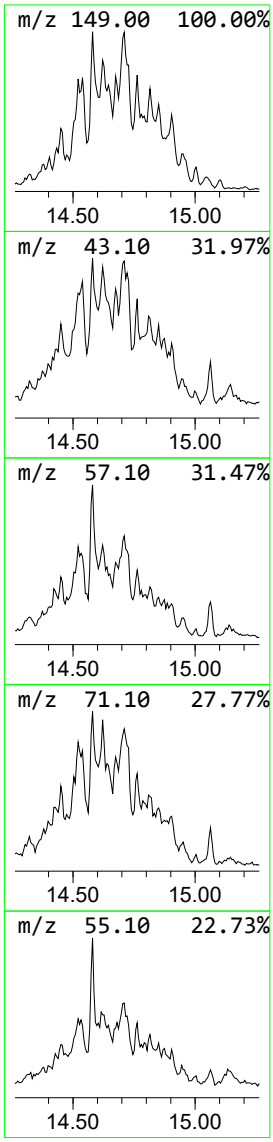
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Phthalic acid, cycloheptyl ... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.762	2.75 ng	93889	Perylene-d12	15.409

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic acid, cycloheptyl nonyl...	388	C24H36O4	1000322-83-4	53
2	Phthalic acid, nonyl trans-hex-3...	374	C23H34O4	1000360-48-7	50
3	1,2-Benzenedicarboxylic acid, de...	418	C26H42O4	000119-07-3	50
4	Phthalic acid, 5-ethyl-1,3-dioxa...	420	C24H36O6	1000415-48-5	50
5	Phthalic acid, decyl 3-methylbut...	374	C23H34O4	1000357-10-8	47





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Data File : BF135289.D
Acq On : 15 Sep 2023 20:26
Operator : CG\JU
Sample : 04399-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11930

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

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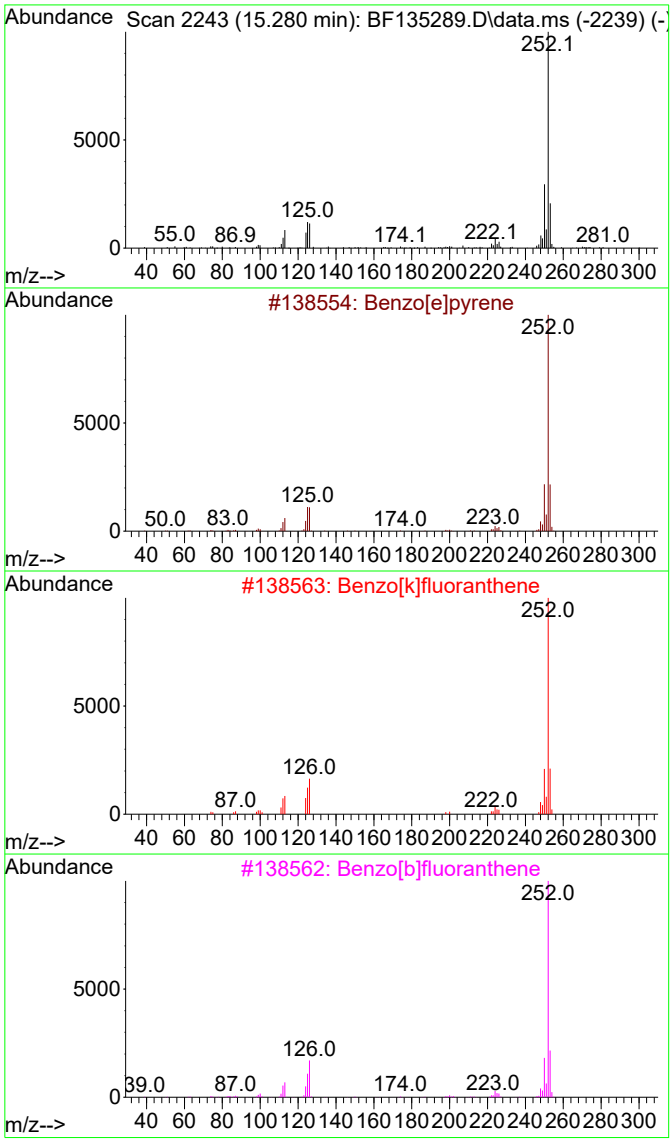
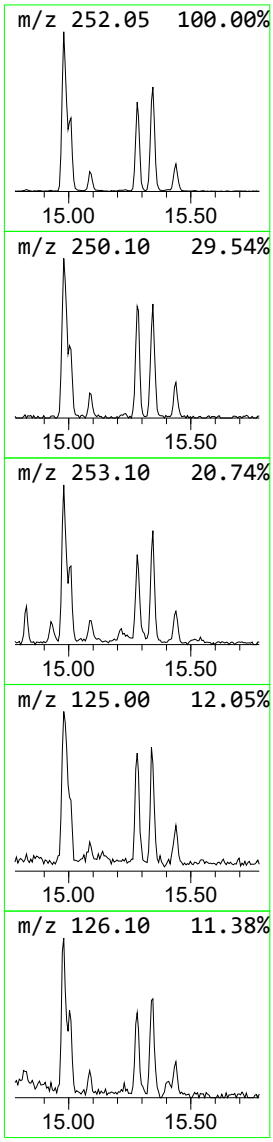
Peak Number 11 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.280	4.14 ng	141133	Perylene-d12	15.409

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	98
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
4	Benzo[a]pyrene	252	C20H12	000050-32-8	95
5	Perylene	252	C20H12	000198-55-0	95





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Operator : CG\JU
Sample : 04399-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11930

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

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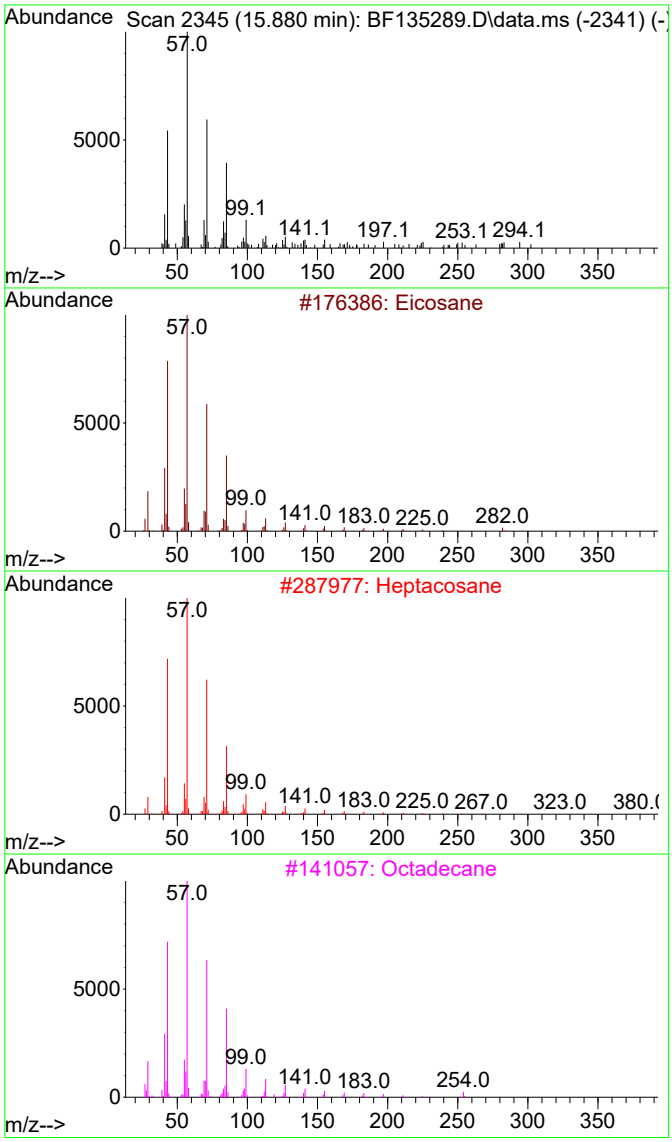
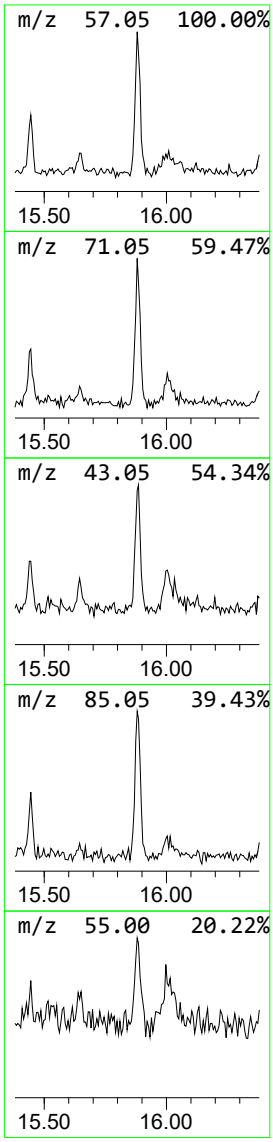
Peak Number 12 Eicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.880	2.31 ng	78725	Perylene-d12	15.409

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	96
2	Heptacosane	380	C27H56	000593-49-7	87
3	Octadecane	254	C18H38	000593-45-3	83
4	Heptadecane	240	C17H36	000629-78-7	83
5	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091523\
Data File : BF135289.D
Acq On : 15 Sep 2023 20:26
Operator : CG\JU
Sample : 04399-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11930

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
2-Pentanone, 4-...	5.010	2.5	ng	85858	1	6.757	674732	20.0
n-Hexadecanoic ...	11.821	5.1	ng	209631	4	11.286	820139	20.0
n-Tetracosanol-1	13.821	2.5	ng	141615	5	13.939	1144080	20.0
Chrysene, 5-met...	14.327	2.8	ng	159320	5	13.939	1144080	20.0
Phthalic acid, ...	14.521	3.3	ng	188507	5	13.939	1144080	20.0
1,4-Benzenedica...	14.580	10.0	ng	573380	5	13.939	1144080	20.0
Phthalic acid, ...	14.621	4.2	ng	242221	5	13.939	1144080	20.0
Phthalic acid, ...	14.674	4.0	ng	138144	6	15.409	682137	20.0
Phthalic acid, ...	14.709	11.0	ng	375003	6	15.409	682137	20.0
Phthalic acid, ...	14.762	2.8	ng	93889	6	15.409	682137	20.0
Benzo[e]pyrene	15.280	4.1	ng	141133	6	15.409	682137	20.0
Eicosane	15.880	2.3	ng	78725	6	15.409	682137	20.0