LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061221\
Data File : BF124285.D
Acq On : 12 Jun 2021 14:33
Operator : JU/CG
Sample : M2651-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 17-B2(0-5)

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-BF060321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124285.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	12	16	20	rBB2	11913	15422	1.67%	0.199%
2	5.045	500	503	510	rVB	32609	39830	4.31%	0.513%
3	5.463	571	574	582	rBV	760790	696455	75.32%	8.974%
4	6.481	742	747	755	rBV	783193	717619	77.61%	9.247%
5	6.669	777	779	787	rBB	15768	16149	1.75%	0.208%
6	6.839	804	808	811	rBV	287448	221782	23.98%	2.858%
7	7.398	899	903	907	rBV	501823	474567	51.32%	6.115%
8	8.122	1022	1026	1033	rBV	368093	286942	31.03%	3.697%
9	9.198	1205	1209	1212	rBV	1230944	924693	100.00%	11.915%
10	9.592	1272	1276	1279	rBV	192072	147393	15.94%	1.899%
11	9.874	1321	1324	1328	rBV	374650	339511	36.72%	4.375%
12	10.669	1455	1459	1462	rBV	643016	577228	62.42%	7.438%
13	11.363	1573	1577	1580	rBV	369237	317704	34.36%	4.094%
14	11.386	1580	1581	1584	rVB	51797	31658	3.42%	0.408%
15	11.892	1664	1667	1671	rBV2	83769	78808	8.52%	1.016%
16	11.974	1679	1681	1684	rBV3	16365	16618	1.80%	0.214%
17	12.504	1767	1771	1777	rVB6	8354	16669	1.80%	0.215%
18	12.580	1780	1784	1787	rBV	181808	152730	16.52%	1.968%
19	12.674	1797	1800	1804	rBV3	34137	32840	3.55%	0.423%
20	12.810	1817	1823	1829	rVB	157486	164156	17.75%	2.115%
21	12.951	1841	1847	1850	rBV	808443	718410	77.69%	9.257%
22	13.027	1855	1860	1864	rBV7	16408	24132	2.61%	0.311%
23	13.139	1875	1879	1882	rVB3	25516	33953	3.67%	0.438%
24	13.204	1887	1890	1893	rVV	22437	21229	2.30%	0.274%
25	13.239	1893	1896	1900	rVV5	15143	17772	1.92%	0.229%
26	13.427	1923	1928	1934	rBV	101947	103409	11.18%	1.333%
27	13.651	1963	1966	1969	rVB4	16676	16961	1.83%	0.219%
28	13.757	1980	1984	1986	rBV4	17642	21942	2.37%	0.283%
29	13.810	1991	1993	1995	rVV	15982	15105	1.63%	0.195%
30	13.857	1998	2001	2010	rVV5	61797	117015	12.65%	1.508%
31	14.010	2019	2027	2029	rBV2	328260	411588	44.51%	5.304%
32	14.033	2029	2031	2037	rVB	94380	90814	9.82%	1.170%
33	14.115	2042	2045	2047	rVB	22692	19166	2.07%	0.247%
34	14.157	2050	2052	2055	rVB4	12982	13034	1.41%	0.168%
35	14.392	2090	2092	2096	rVB3	21673	18606	2.01%	0.240%
36	14.498	2107	2110	2111	rBV3	15171	15033	1.63%	0.194%

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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 17-B2(0-5)

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.521	2111	2114	2115	rBV3	20488	17772	1.92%	0.229%
38	14.780	2156	2158	2161	rBV4	18428	16978	1.84%	0.219%
39	15.057	2201	2205	2208	rBV	102469	154443	16.70%	1.990%
40	15.115	2212	2215	2219	rBV6	21248	35709	3.86%	0.460%
41	15.162	2221	2223	2226	rBV3	25763	23398	2.53%	0.302%
42	15.356	2253	2256	2261	rVB2	51781	78324	8.47%	1.009%
43	15.421	2263	2267	2271	rVV	84787	102477	11.08%	1.320%
44	15.486	2274	2278	2287	rVB	186676	270478	29.25%	3.485%
45	16.256	2407	2409	2416	rVB7	11762	16259	1.76%	0.210%
46	16.962	2525	2529	2535	rVB5	29679	58244	6.30%	0.751%
47	17.198	2567	2569	2573	rVB5	13674	17018	1.84%	0.219%
48	17.409	2601	2605	2611	rVB6	20073	42427	4.59%	0.547%

Sum of corrected areas: 7760470

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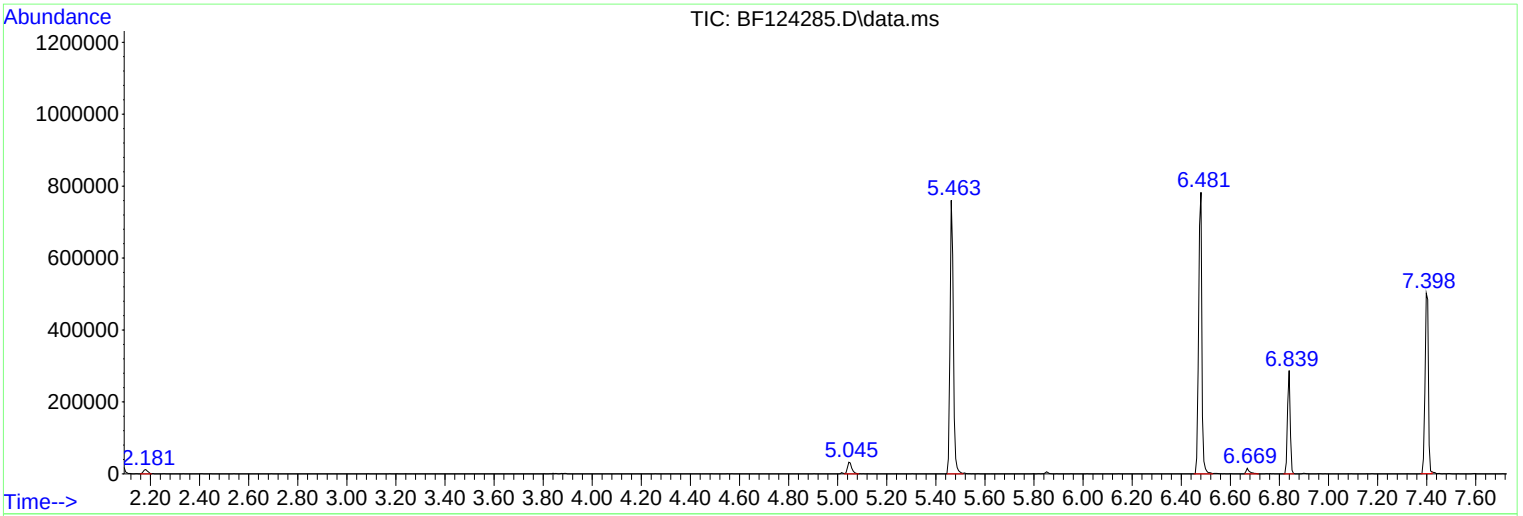
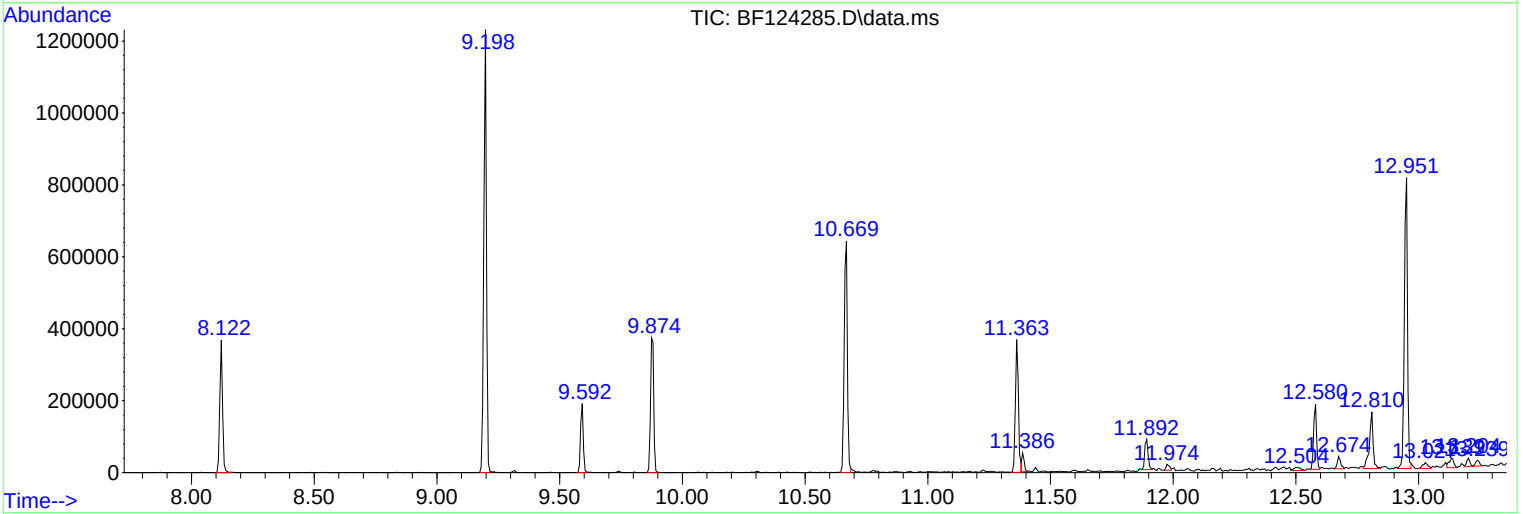
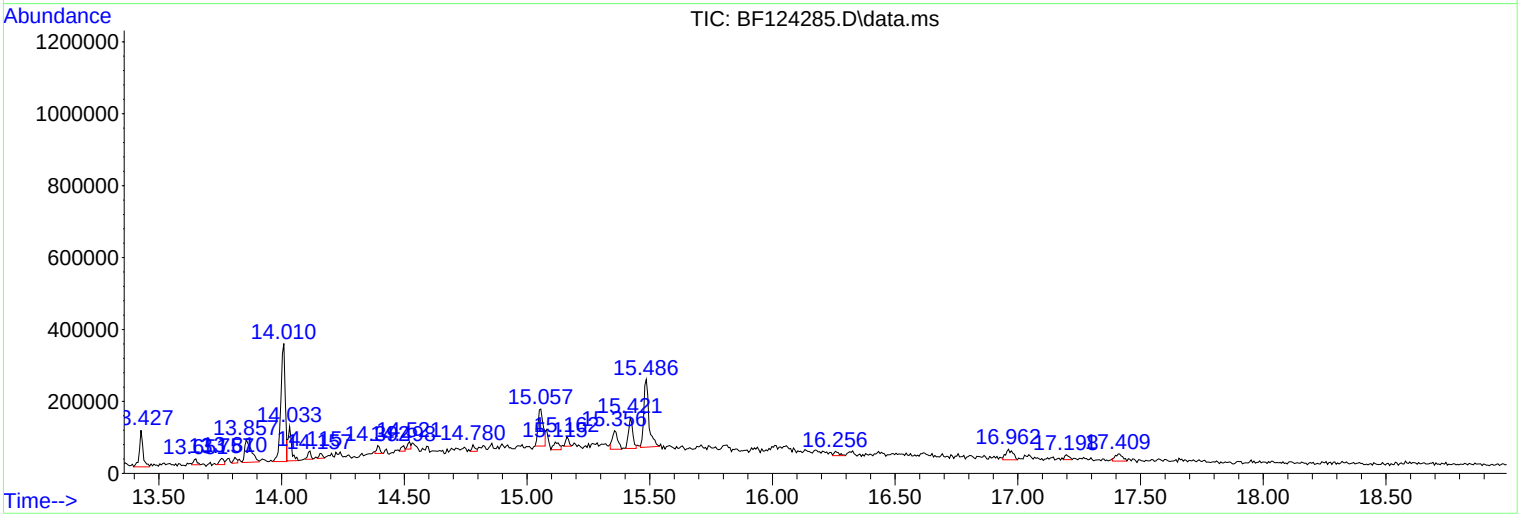
Instrument :
BNA_F
ClientSampleId :
17-B2(0-5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P







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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
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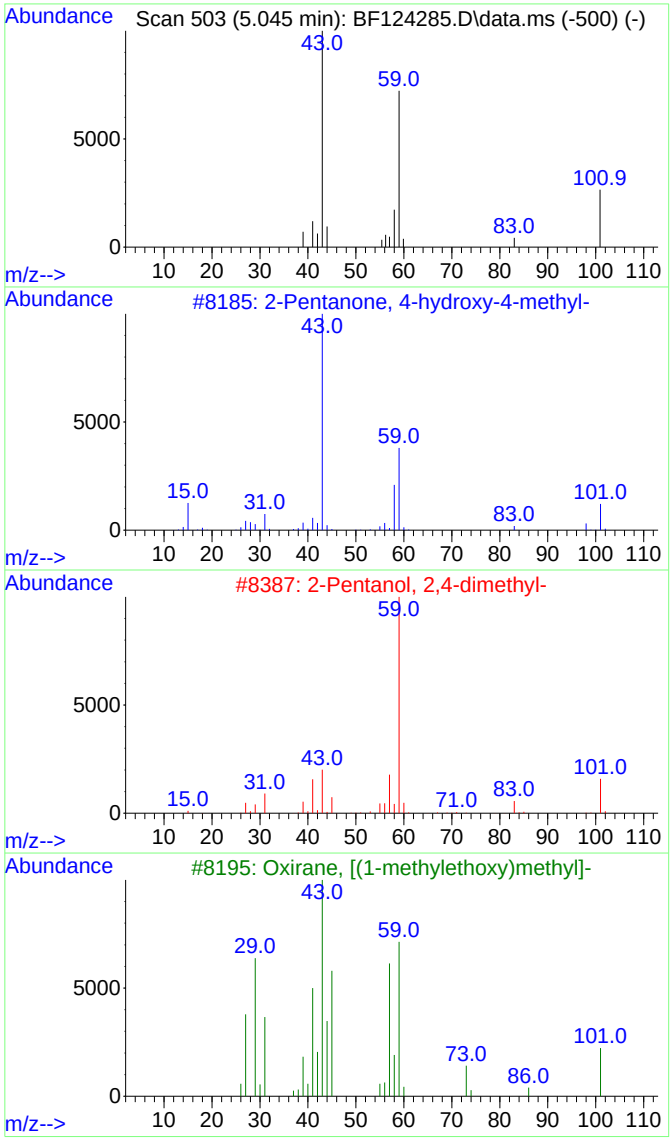
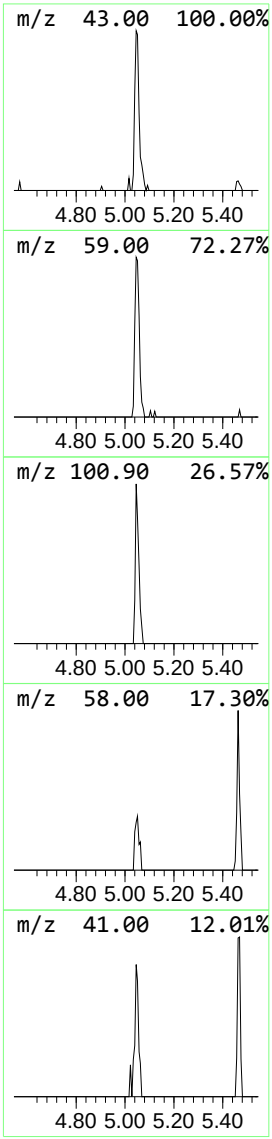
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.045	3.59 ng	39830	1,4-Dichlorobenzene-d4	6.839

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	42
3	Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	39
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	25
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Instrument :
BNA_F
ClientSampleId :
17-B2(0-5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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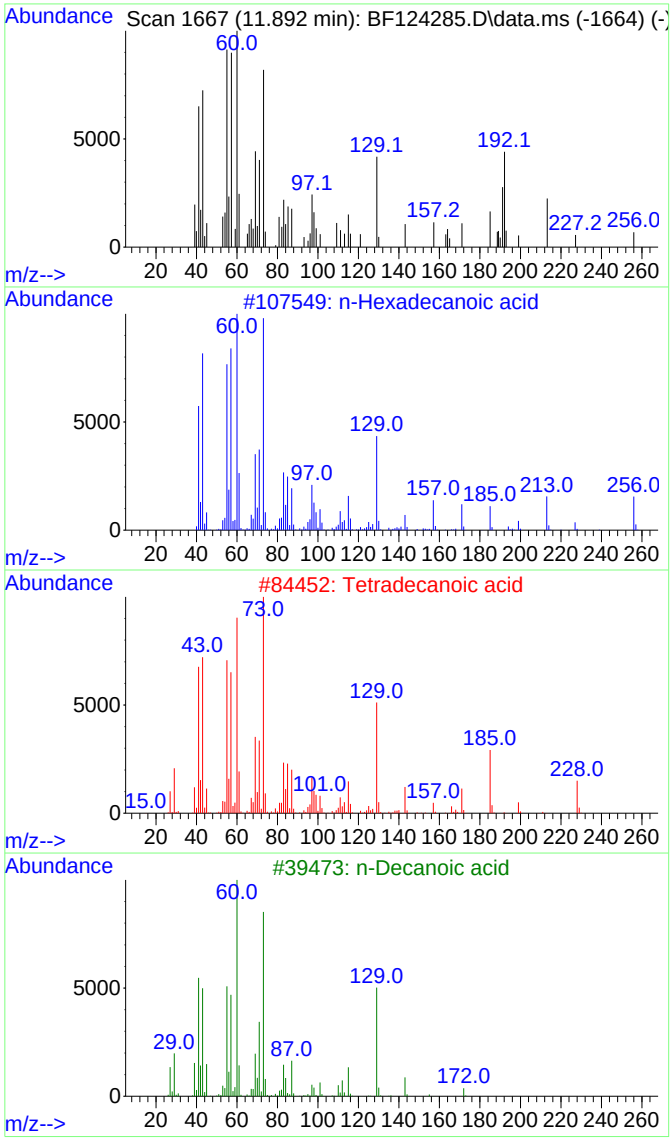
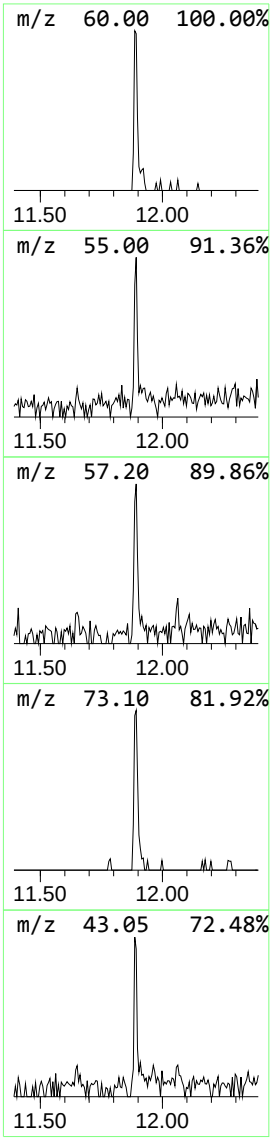
Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	4.96 ng	78808	Phenanthrene-d10	11.363

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	62
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
3	n-Decanoic acid	172	C10H20O2	000334-48-5	49
4	Tridecanoic acid	214	C13H26O2	000638-53-9	47
5	Dodecanoic acid	200	C12H24O2	000143-07-7	47





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Operator : JU/CG
Sample : M2651-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 17-B2(0-5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
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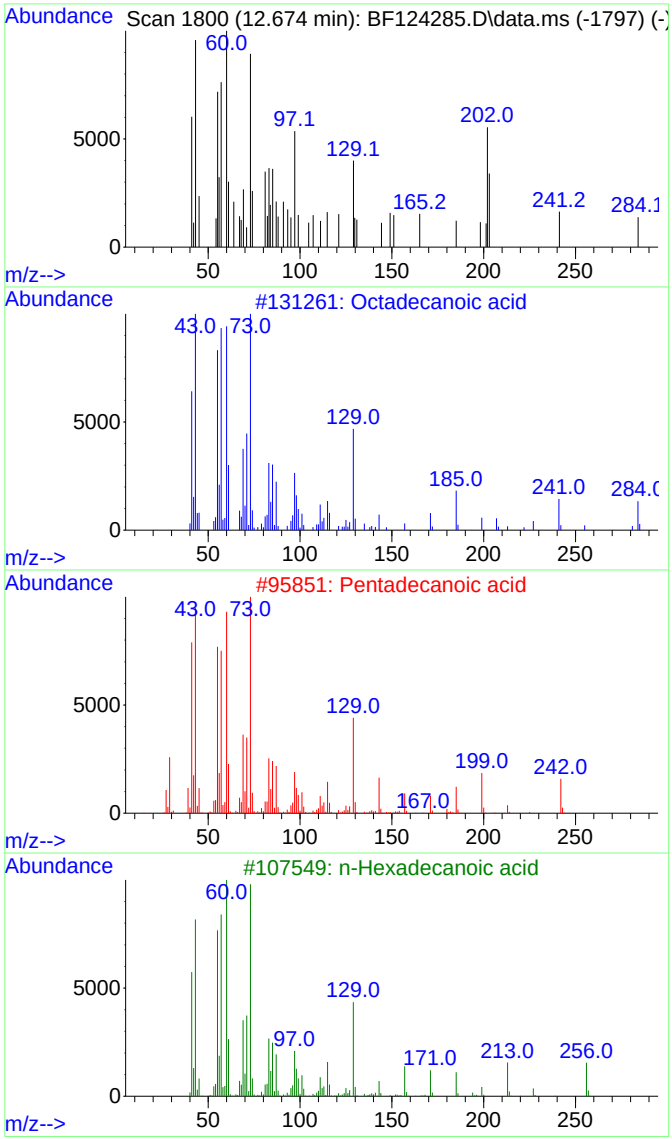
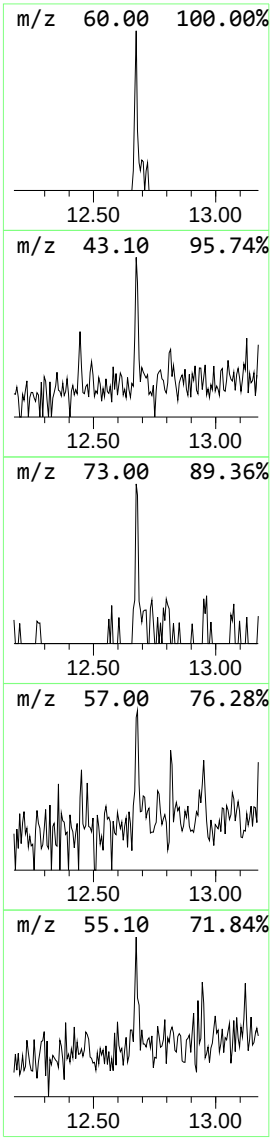
Peak Number 3 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.674	2.07 ng	32840	Phenanthrene-d10	11.363

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	91
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	47
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	47
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	47
5	Dodecanoic acid	200	C12H24O2	000143-07-7	38





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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 17-B2(0-5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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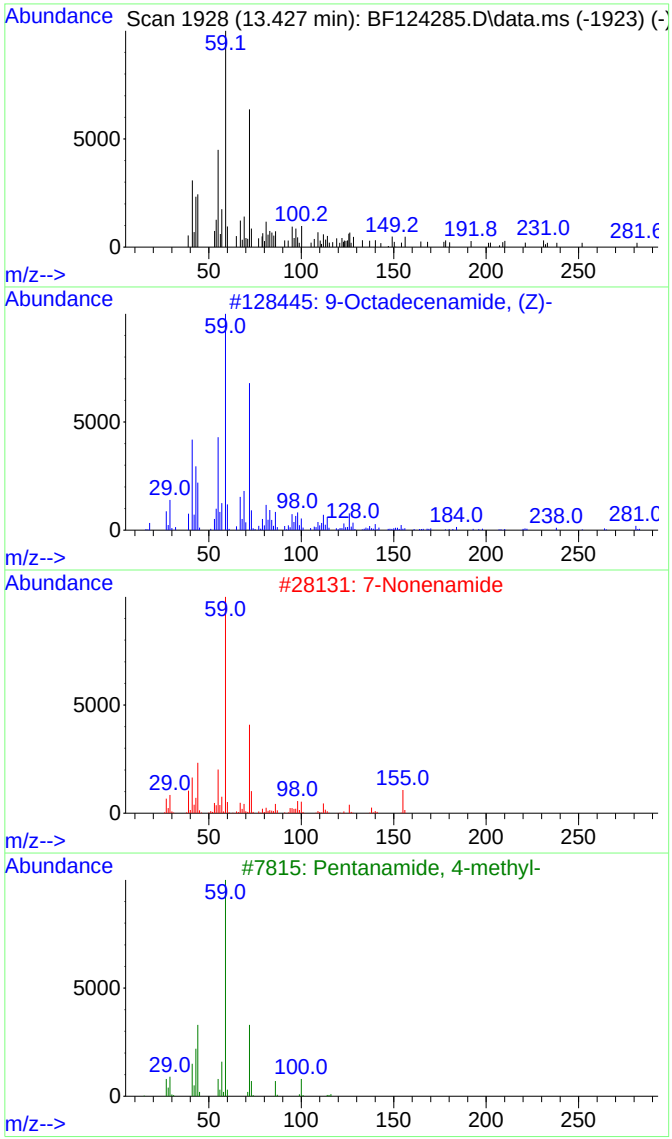
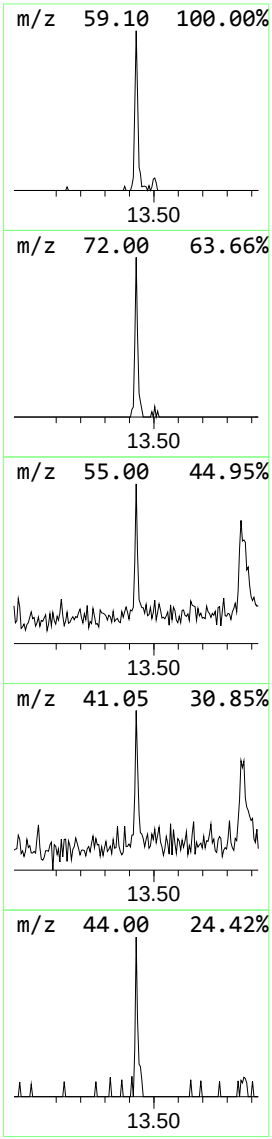
Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.427	5.02 ng	103409	Chrysene-d12	14.009

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	94
2	7-Nonenamide	155	C9H17NO	090949-53-4	53
3	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	50
4	Dodecanamide	199	C12H25NO	001120-16-7	50
5	Hexadecanamide	255	C16H33NO	000629-54-9	47





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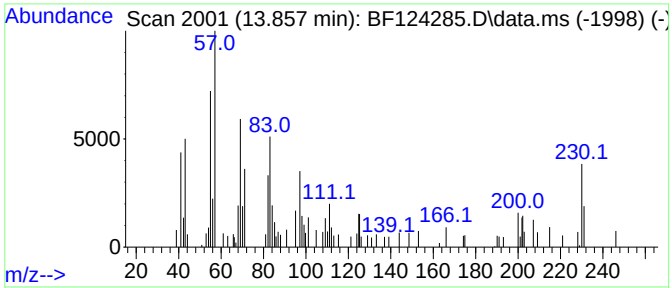
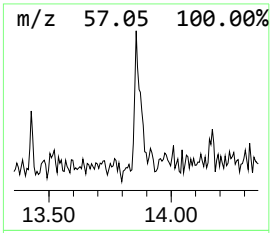
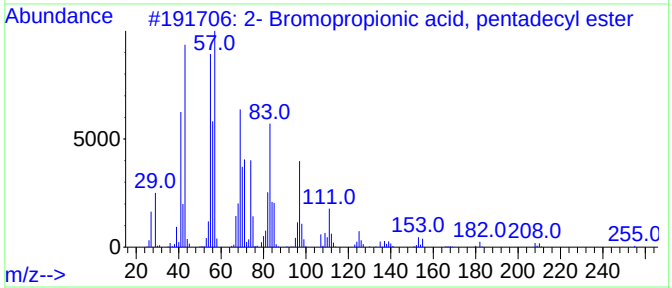
Peak Number 5 unknown13.857 Concentration Rank 2

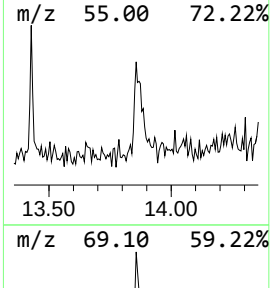
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	5.69 ng	117015	Chrysene-d12	14.009

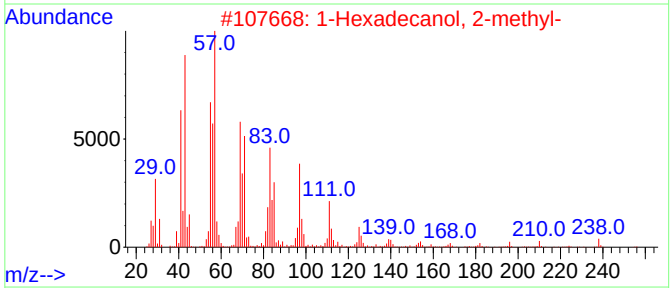
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Bromopropionic acid, pentadec...	362	C18H35BrO2	1000292-44-2	43
2	1-Hexadecanol, 2-methyl-	256	C17H36O	002490-48-4	43
3	Cyclopentane, undecyl-	224	C16H32	006785-23-5	43
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	43
5	1-Hentetracontanol	593	C41H84O	040710-42-7	38

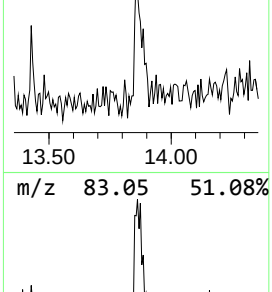


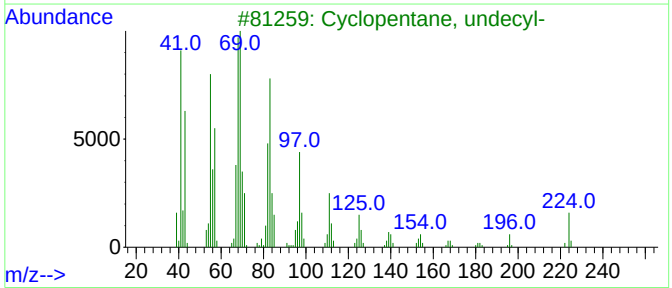












Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.045	3.6	ng	39830	1	6.839	221782	20.0
n-Hexadecanoic ...	11.892	5.0	ng	78808	4	11.363	317704	20.0
Octadecanoic acid	12.674	2.1	ng	32840	4	11.363	317704	20.0
9-Octadecenamid...	13.427	5.0	ng	103409	5	14.009	411588	20.0
unknown13.857	13.857	5.7	ng	117015	5	14.009	411588	20.0