

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060921\
 Data File : BF124211.D
 Acq On : 9 Jun 2021 16:23
 Operator : JU/CG
 Sample : M2624-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 G-1

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: BF124211.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.475	573	576	580	rBV	945667	907769	80.61%	10.531%
2	6.492	744	749	752	rBV	1005541	928518	82.45%	10.772%
3	6.845	806	809	813	rBV	293635	224083	19.90%	2.600%
4	7.410	901	905	908	rBV	714438	639487	56.79%	7.419%
5	8.033	1008	1011	1015	rBV	16566	17265	1.53%	0.200%
6	8.128	1023	1027	1030	rBV	347662	279742	24.84%	3.245%
7	9.204	1206	1210	1213	rBV	1285060	1126098	100.00%	13.064%
8	9.522	1261	1264	1266	rBV2	39530	30381	2.70%	0.352%
9	9.598	1274	1277	1280	rBV	39214	28757	2.55%	0.334%
10	9.886	1322	1326	1329	rVB	444082	344345	30.58%	3.995%
11	10.674	1456	1460	1464	rBV	971669	819727	72.79%	9.510%
12	11.374	1575	1579	1581	rBV	344329	330059	29.31%	3.829%
13	11.392	1581	1582	1586	rVV	129669	91199	8.10%	1.058%
14	11.445	1589	1591	1594	rVB	19398	15248	1.35%	0.177%
15	11.874	1660	1664	1665	rBV3	11762	12609	1.12%	0.146%
16	11.898	1665	1668	1672	rVV2	64928	60782	5.40%	0.705%
17	11.986	1680	1683	1685	rBV2	13388	16101	1.43%	0.187%
18	12.192	1716	1718	1721	rVB2	19521	16846	1.50%	0.195%
19	12.586	1781	1785	1788	rBV	174425	142390	12.64%	1.652%
20	12.680	1798	1801	1804	rBV3	16869	15357	1.36%	0.178%
21	12.815	1817	1824	1829	rVB	118850	127478	11.32%	1.479%
22	12.957	1844	1848	1851	rBV	990971	786004	69.80%	9.119%
23	13.039	1856	1862	1865	rVB6	10062	16539	1.47%	0.192%
24	13.139	1876	1879	1884	rVB3	18788	22797	2.02%	0.264%
25	13.274	1899	1902	1905	rVB4	10393	13010	1.16%	0.151%
26	13.386	1916	1921	1924	rBV5	78510	81460	7.23%	0.945%
27	13.421	1924	1927	1931	rVB5	30974	40044	3.56%	0.465%
28	13.651	1962	1966	1969	rBV2	13033	15733	1.40%	0.183%
29	13.757	1981	1984	1987	rBV4	15196	18089	1.61%	0.210%
30	13.862	1999	2002	2003	rBV2	22040	22872	2.03%	0.265%
31	14.010	2022	2027	2030	rBV2	272945	320366	28.45%	3.717%
32	14.039	2030	2032	2034	rVB	65565	49049	4.36%	0.569%
33	14.139	2047	2049	2051	rVB3	14656	13563	1.20%	0.157%
34	14.180	2054	2056	2058	rVV3	25492	19058	1.69%	0.221%
35	14.209	2058	2061	2063	rVV4	15496	20880	1.85%	0.242%
36	14.233	2063	2065	2069	rVB5	18648	20791	1.85%	0.241%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060921\
 Data File : BF124211.D
 Acq On : 9 Jun 2021 16:23
 Operator : JU/CG
 Sample : M2624-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 G-1

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

37	14.404	2090	2094	2097	rBV5	13515	18433	1.64%	0.214%
38	14.474	2103	2106	2108	rBV4	13981	15591	1.38%	0.181%
39	14.521	2112	2114	2121	rVB8	20795	28494	2.53%	0.331%
40	14.862	2168	2172	2174	rBV2	36459	32955	2.93%	0.382%
41	15.056	2202	2205	2208	rBV2	69136	93109	8.27%	1.080%
42	15.121	2213	2216	2221	rVB5	27522	31682	2.81%	0.368%
43	15.362	2254	2257	2263	rVB3	40340	53888	4.79%	0.625%
44	15.427	2263	2268	2272	rBV	53504	69423	6.16%	0.805%
45	15.486	2273	2278	2286	rBV2	204117	304678	27.06%	3.535%
46	15.945	2351	2356	2363	rVB8	30428	57173	5.08%	0.663%
47	16.015	2365	2368	2371	rVV4	9454	14242	1.26%	0.165%
48	16.062	2375	2376	2380	rVB4	12441	12770	1.13%	0.148%
49	16.192	2394	2398	2403	rVB8	14690	25943	2.30%	0.301%
50	16.774	2494	2497	2499	rVB3	12159	12326	1.09%	0.143%
51	16.968	2525	2530	2535	rBV9	24677	47997	4.26%	0.557%
52	17.045	2541	2543	2549	rVB6	20773	28009	2.49%	0.325%
53	17.121	2553	2556	2560	rBV6	8737	15568	1.38%	0.181%
54	17.580	2628	2634	2636	rBV7	9536	15526	1.38%	0.180%
55	18.109	2720	2724	2730	rVB9	16121	33232	2.95%	0.386%
56	18.192	2735	2738	2742	rBV5	7689	12569	1.12%	0.146%
57	18.245	2744	2747	2749	rBV3	12010	13940	1.24%	0.162%
58	18.274	2749	2752	2756	rVB6	12364	18166	1.61%	0.211%
59	18.392	2766	2772	2774	rBV6	10895	15804	1.40%	0.183%
60	18.586	2800	2805	2808	rBV5	7654	13857	1.23%	0.161%

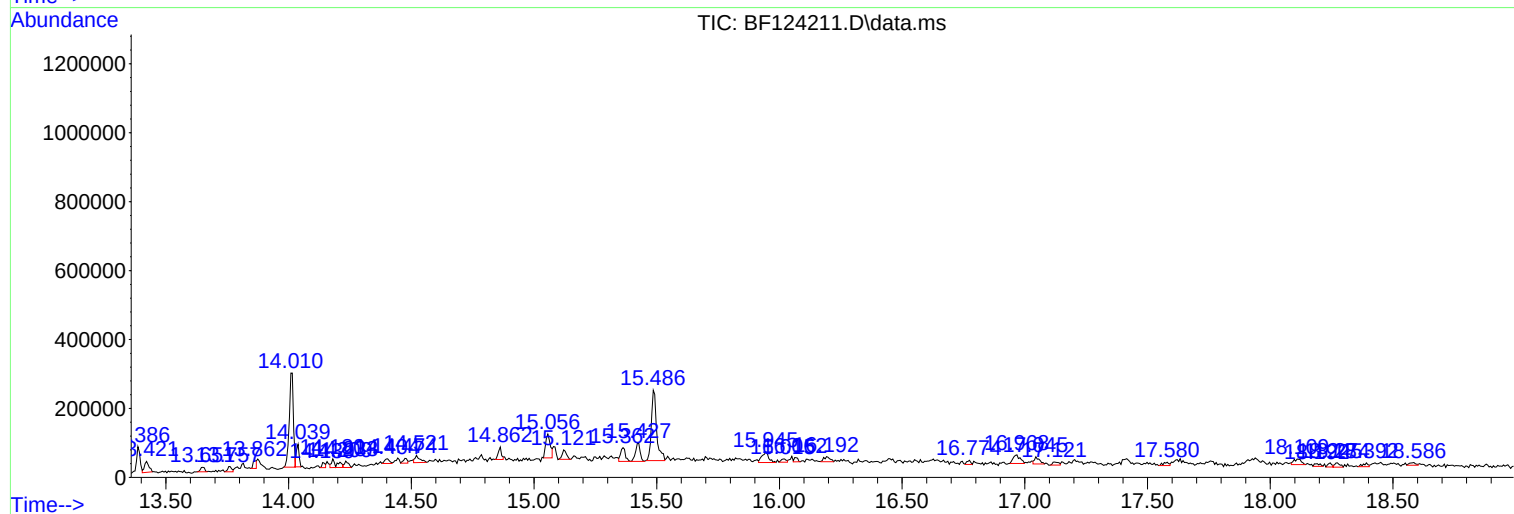
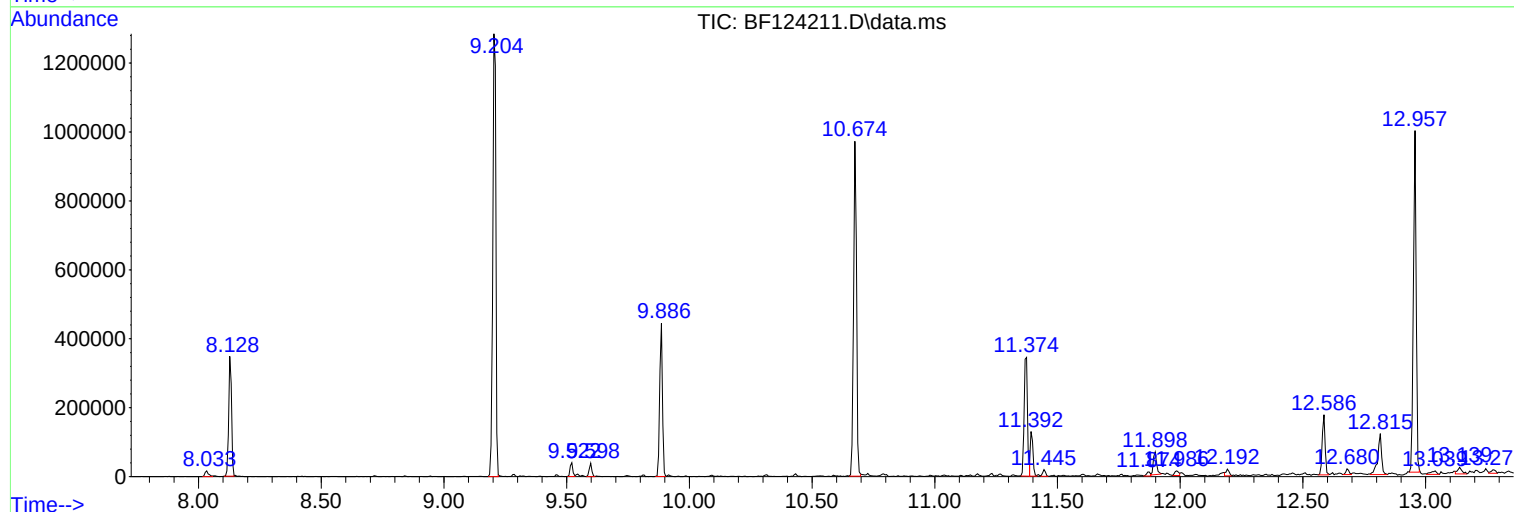
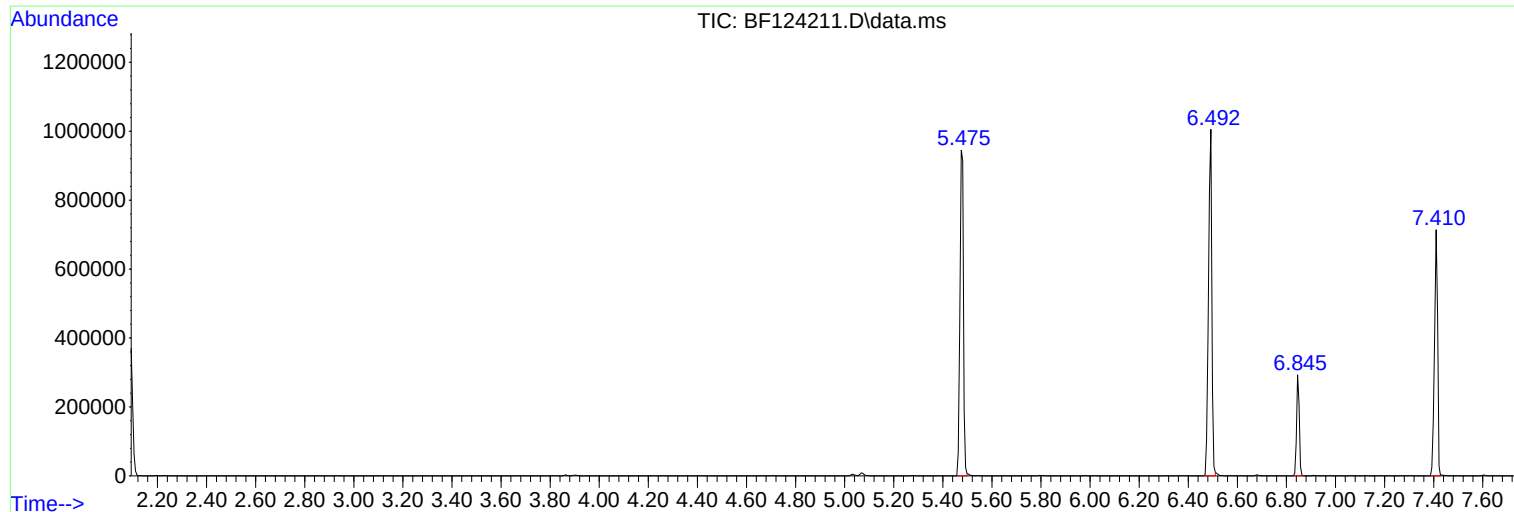
Sum of corrected areas: 8619871

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060921\
Data File : BF124211.D
Acq On : 9 Jun 2021 16:23
Operator : JU/CG
Sample : M2624-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
G-1

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060921\
Data File : BF124211.D
Acq On : 9 Jun 2021 16:23
Operator : JU/CG
Sample : M2624-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
G-1

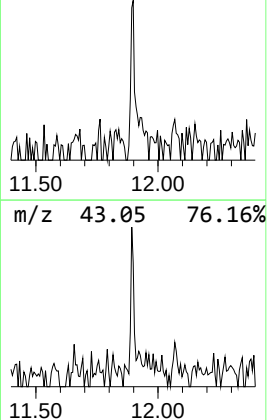
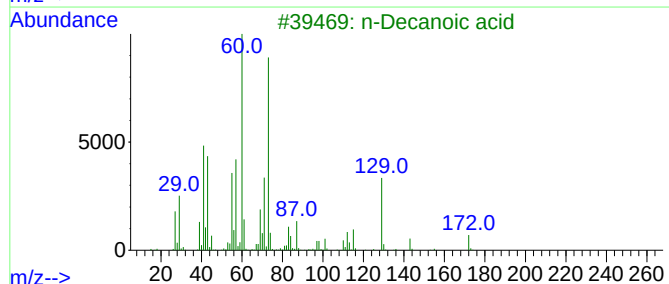
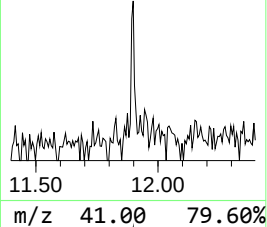
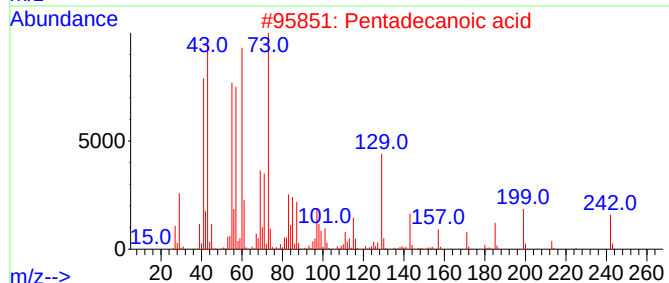
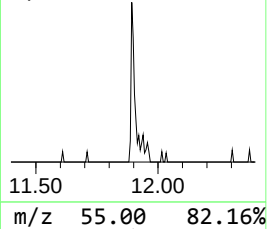
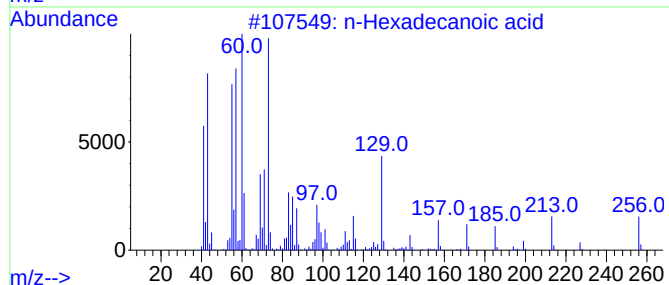
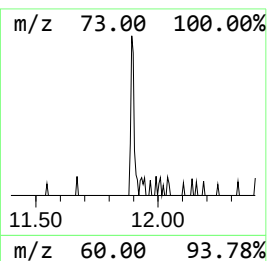
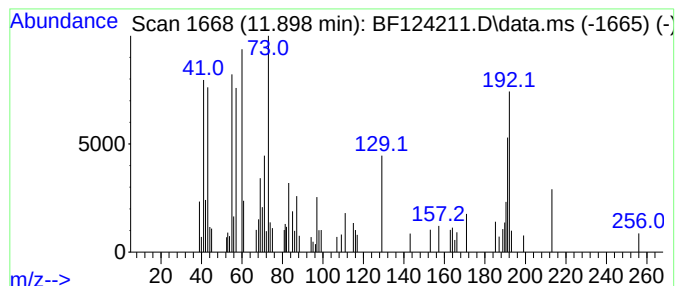
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	3.68 ng	60782	Phenanthrene-d10	11.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	46
3			n-Decanoic acid	172	C10H20O2	000334-48-5	38
4			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	35
5			Silver butanoate	194	C4H7AgO2	005076-24-4	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060921\
Data File : BF124211.D
Acq On : 9 Jun 2021 16:23
Operator : JU/CG
Sample : M2624-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
G-1

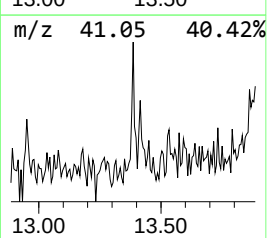
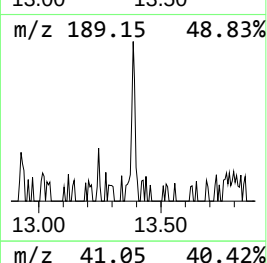
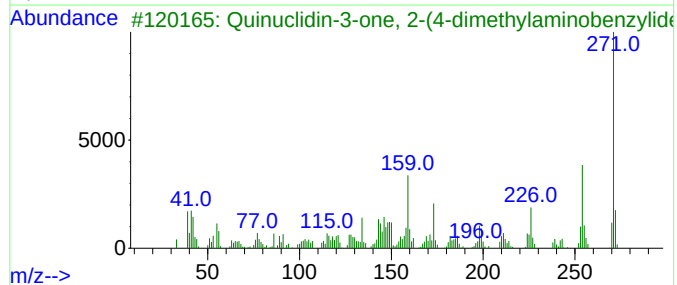
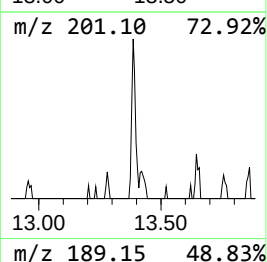
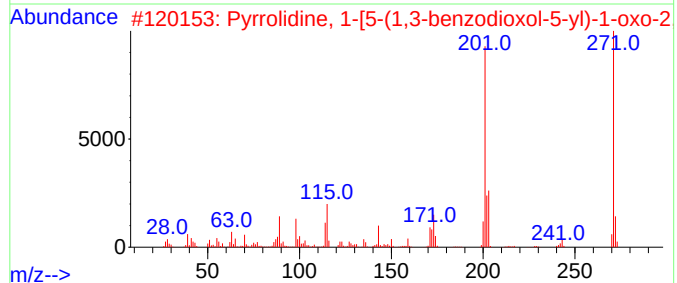
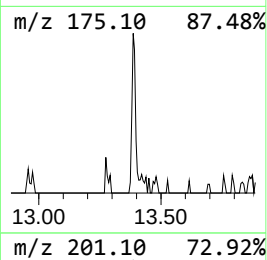
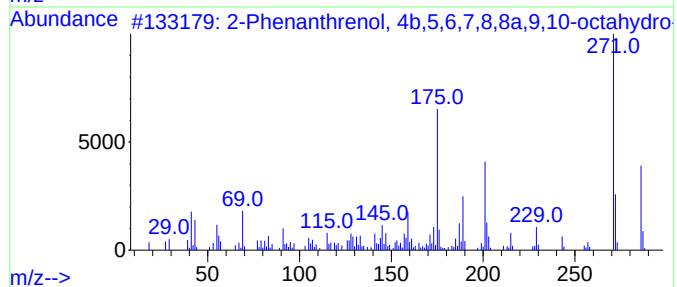
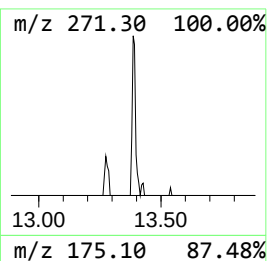
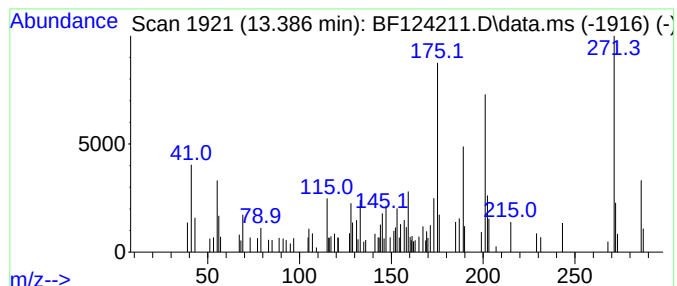
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.386	5.09 ng	81460	Chrysene-d12	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	94		
2	Pyrrolidine, 1-[5-(1,3-benzodiox...	271	C16H17NO3	025924-78-1	22		
3	Quinuclidin-3-one, 2-(4-dimethyl...	271	C16H21N3O	1000266-14-6	22		
4	Methanone, (2-chloro-4,5-difluor...	287	C14H16ClF2NO	1000277-48-2	18		
5	Oxazole, 2-(1-naphthalenyl)-5-ph...	271	C19H13NO	000846-63-9	11		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060921\
Data File : BF124211.D
Acq On : 9 Jun 2021 16:23
Operator : JU/CG
Sample : M2624-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
G-1

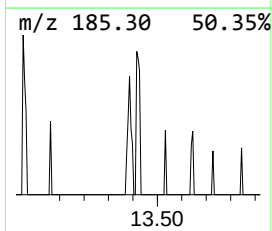
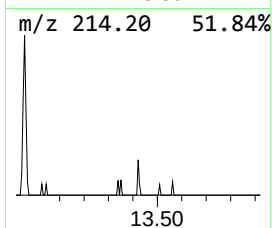
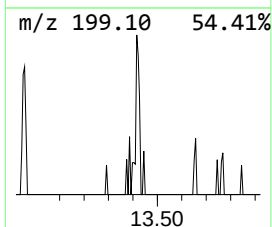
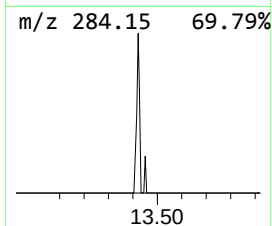
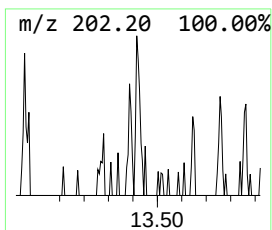
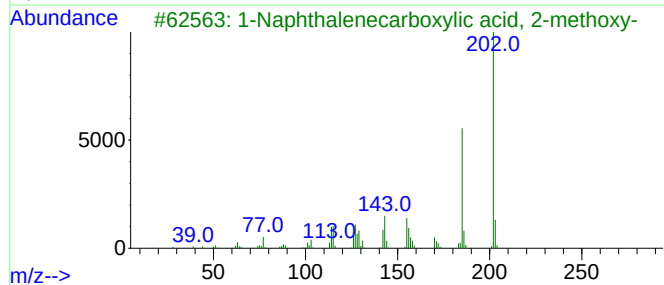
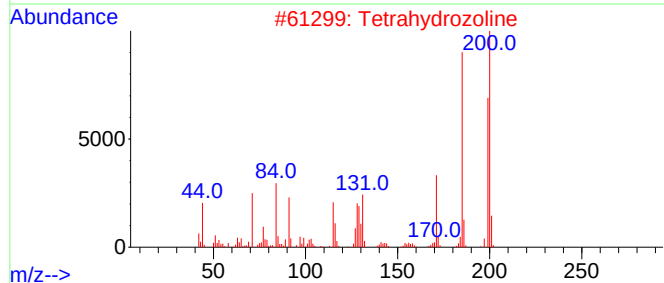
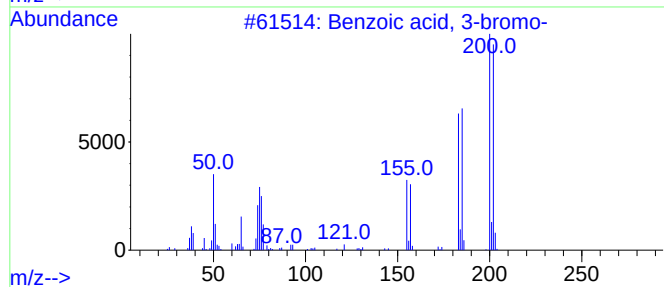
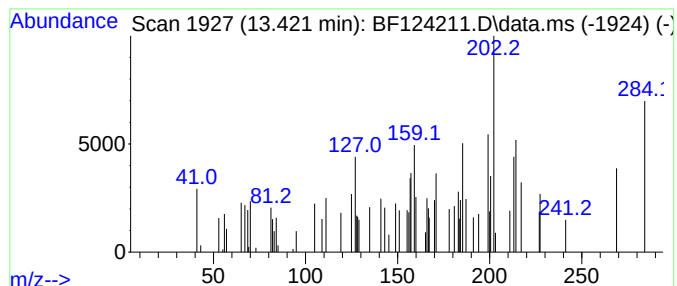
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown13.421 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.421	2.50 ng	40044	Chrysene-d12	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 3-bromo-	200	C7H5BrO2	000585-76-2	18
2			Tetrahydrozoline	200	C13H16N2	000084-22-0	18
3			1-Naphthalenecarboxylic acid, 2-...	202	C12H10O3	000947-62-6	14
4			s-Indacene, 1,2,3,5,6,7-hexahydr...	214	C16H22	055030-60-9	14
5			Benzoic acid, 2-bromo-	200	C7H5BrO2	000088-65-3	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060921\
Data File : BF124211.D
Acq On : 9 Jun 2021 16:23
Operator : JU/CG
Sample : M2624-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
G-1

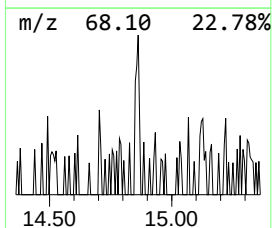
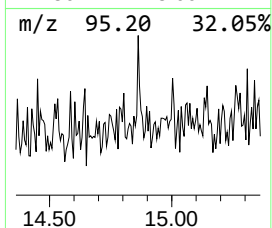
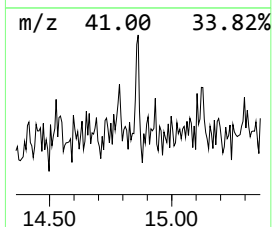
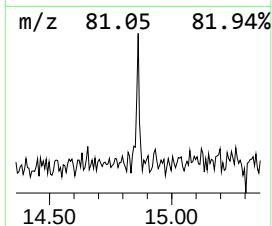
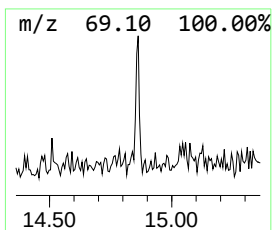
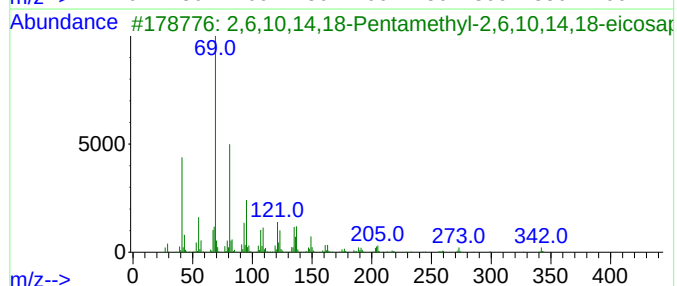
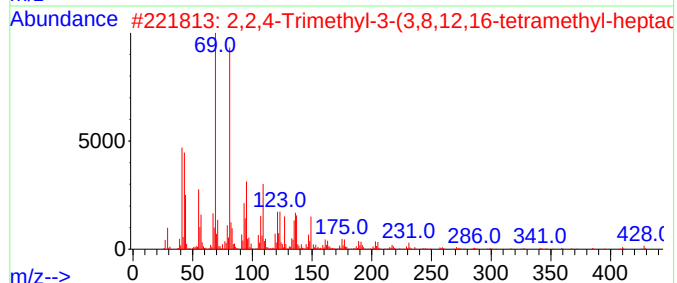
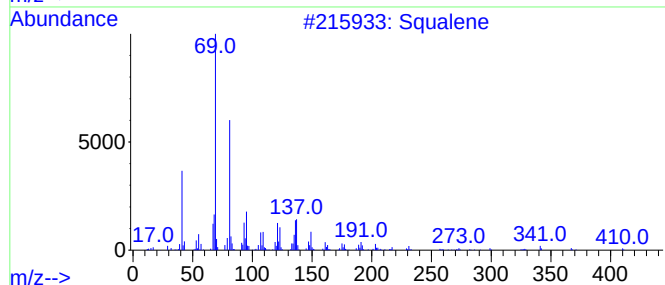
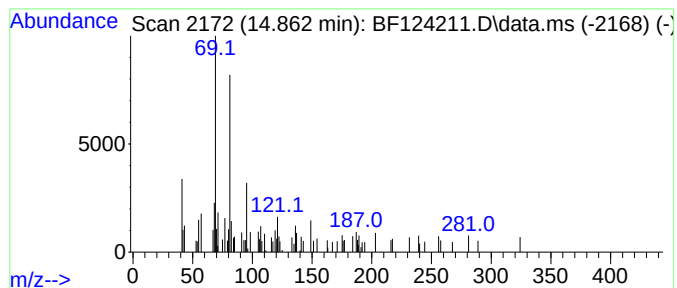
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.862	2.16 ng	32955	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	50
2			2,2,4-Trimethyl-3-(3,8,12,16-tet...	428	C30H52O	1000194-01-4	50
3			2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	38
4			1-Pentadecyne	208	C15H28	000765-13-9	35
5			Hexadeca-2,6,10,14-tetraen-1-ol,...	290	C20H34O	007614-21-3	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060921\
Data File : BF124211.D
Acq On : 9 Jun 2021 16:23
Operator : JU/CG
Sample : M2624-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

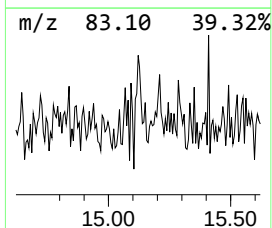
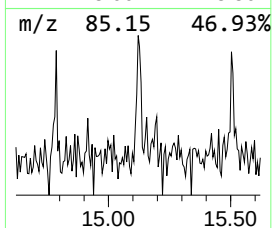
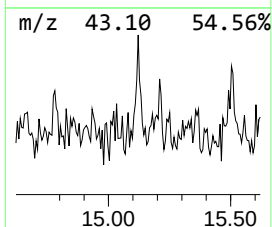
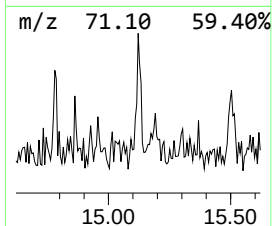
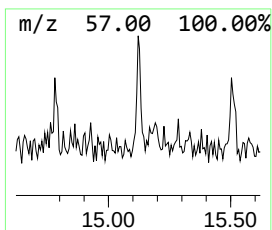
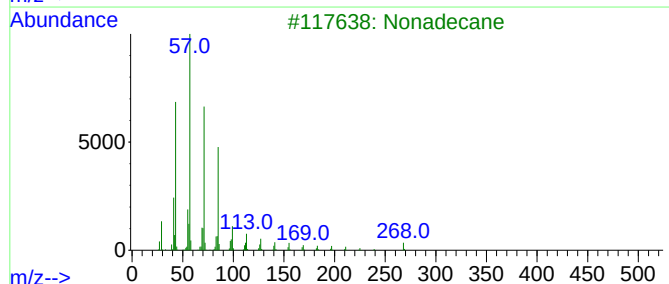
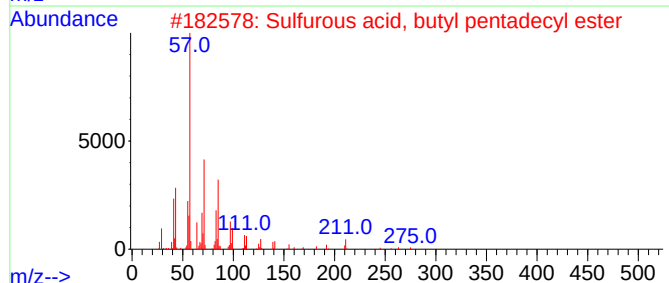
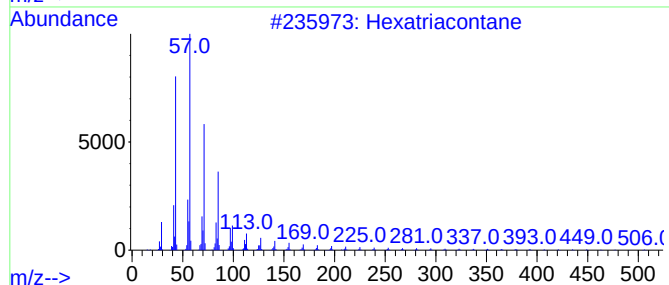
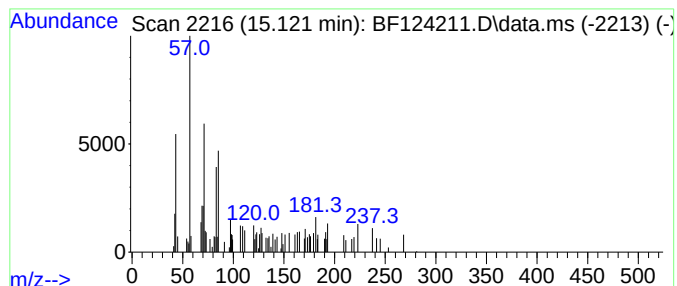
Instrument :
BNA_F
ClientSampleId :
G-1

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

Peak Number 5 unknown15.121 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.121	2.08 ng	31682	Perylene-d12	15.492	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexatriacontane	507	C36H74	000630-06-8	43
2	Sulfurous acid, butyl pentadecyl...	348	C19H40O3S	1000309-18-2	43
3	Nonadecane	268	C19H40	000629-92-5	41
4	Hentriacontane	437	C31H64	000630-04-6	38
5	Dodecane	170	C12H26	000112-40-3	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060921\
Data File : BF124211.D
Acq On : 9 Jun 2021 16:23
Operator : JU/CG
Sample : M2624-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
G-1

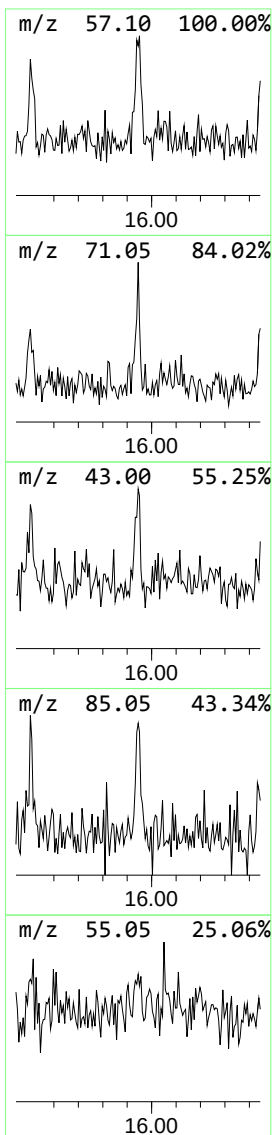
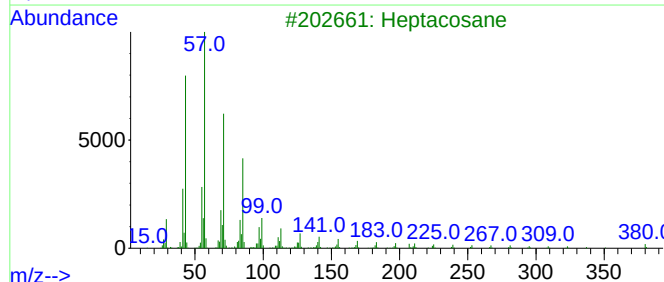
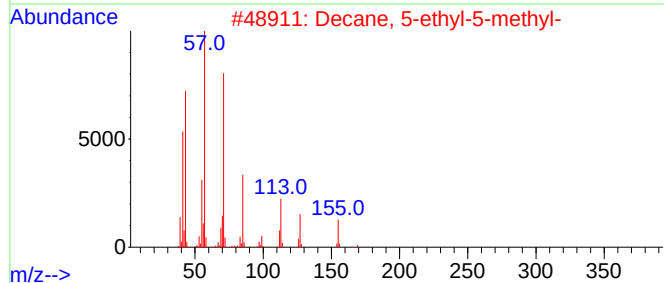
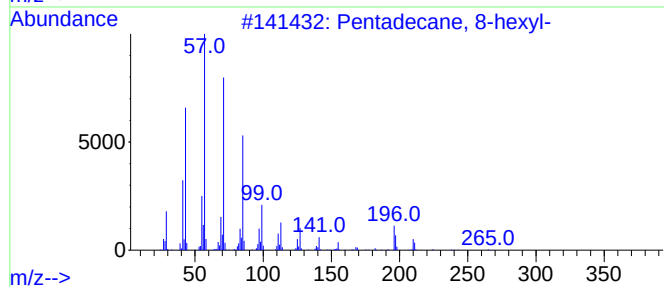
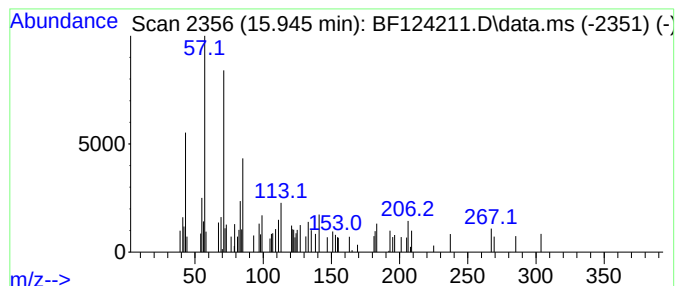
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentadecane, 8-hexyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.945	3.75 ng	57173	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	53
2			Decane, 5-ethyl-5-methyl-	184	C13H28	017312-74-2	53
3			Heptacosane	380	C27H56	000593-49-7	52
4			Decane, 1-bromo-2-methyl-	234	C11H23Br	127839-47-8	50
5			Tridecane	184	C13H28	000629-50-5	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060921\
Data File : BF124211.D
Acq On : 9 Jun 2021 16:23
Operator : JU/CG
Sample : M2624-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
G-1

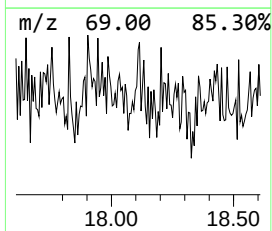
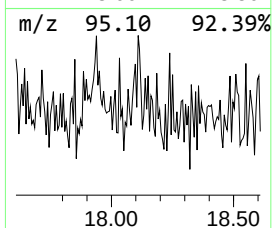
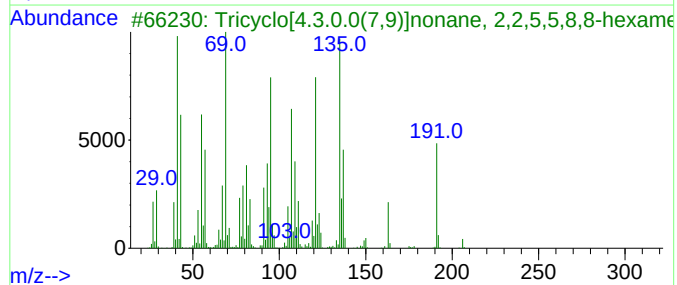
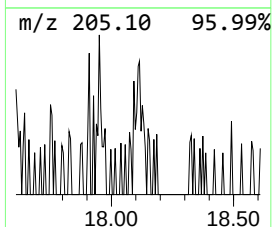
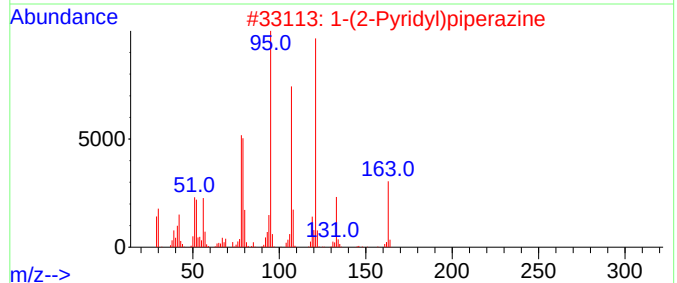
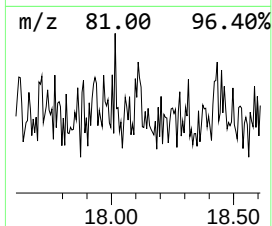
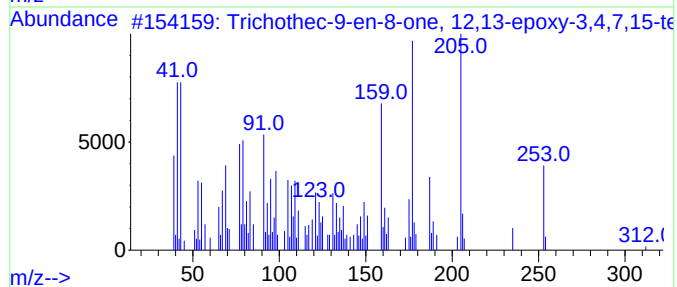
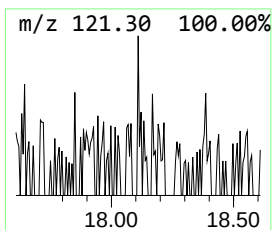
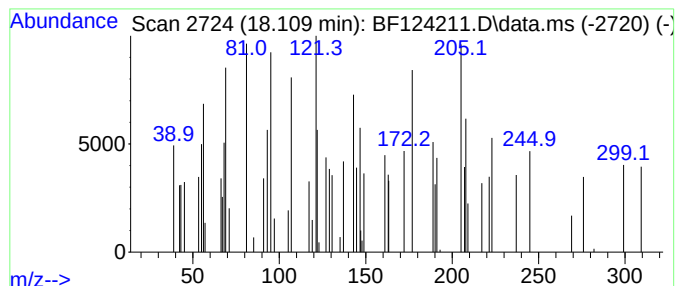
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown18.109 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.109	2.18 ng	33232	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichothec-9-en-8-one, 12,13-epo...	312	C15H20O7	023282-20-4	22
2			1-(2-Pyridyl)piperazine	163	C9H13N3	034803-66-2	22
3			Tricyclo[4.3.0.0(7,9)]nonane, 2,...	206	C15H26	054832-82-5	12
4			1,2,4,5-Tetrazin-3-amine, 6-(3,5...	223	C7H9N7O2	1000277-43-8	11
5			2-Ethylmercapto-4-amino-5-chloro...	205	C6H8ClN3OS	1000253-98-1	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060921\
Data File : BF124211.D
Acq On : 9 Jun 2021 16:23
Operator : JU/CG
Sample : M2624-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
G-1

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	11.898	3.7	ng	60782	4	11.374	330059	20.0
2-Phenanthrenol...	13.386	5.1	ng	81460	5	14.015	320366	20.0
unknown13.421	13.421	2.5	ng	40044	5	14.015	320366	20.0
Squalene	14.862	2.2	ng	32955	6	15.492	304678	20.0
unknown15.121	15.121	2.1	ng	31682	6	15.492	304678	20.0
Pentadecane, 8-...	15.945	3.8	ng	57173	6	15.492	304678	20.0
unknown18.109	18.109	2.2	ng	33232	6	15.492	304678	20.0