

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061221\
 Data File : BF124294.D
 Acq On : 12 Jun 2021 19:23
 Operator : JU/CG
 Sample : M2639-01 2X
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B67

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: BF124294.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	11	15	20	rBB3	7246	9482	1.69%	0.189%
2	5.057	501	505	512	rBB	15918	18438	3.28%	0.367%
3	5.475	573	576	588	rBV	455530	433436	77.19%	8.631%
4	6.492	746	749	762	rBV	398987	422024	75.16%	8.404%
5	6.839	805	808	812	rBV	272429	218573	38.92%	4.353%
6	7.404	900	904	910	rBV	365917	308616	54.96%	6.146%
7	8.122	1023	1026	1035	rVB	261042	243523	43.37%	4.849%
8	9.198	1205	1209	1214	rBV	730661	561526	100.00%	11.182%
9	9.880	1321	1325	1329	rBV	325779	244842	43.60%	4.876%
10	10.669	1456	1459	1464	rBV	292649	274318	48.85%	5.463%
11	11.227	1548	1554	1558	rBV4	15045	17143	3.05%	0.341%
12	11.369	1575	1578	1580	rBV	258712	223638	39.83%	4.453%
13	11.392	1580	1582	1586	rVV	101073	75636	13.47%	1.506%
14	11.445	1588	1591	1596	rVB	20335	16605	2.96%	0.331%
15	11.610	1615	1619	1620	rBV5	7530	7668	1.37%	0.153%
16	11.763	1641	1645	1647	rBV2	8258	7805	1.39%	0.155%
17	11.869	1660	1663	1666	rBV2	15452	18003	3.21%	0.359%
18	11.898	1666	1668	1672	rVV2	31456	34805	6.20%	0.693%
19	11.945	1674	1676	1680	rVV2	11339	15509	2.76%	0.309%
20	11.986	1680	1683	1685	rVV3	20840	24818	4.42%	0.494%
21	12.004	1685	1686	1691	rVB3	13644	13004	2.32%	0.259%
22	12.169	1711	1714	1716	rBV3	10514	10304	1.83%	0.205%
23	12.198	1716	1719	1722	rVB3	12380	12254	2.18%	0.244%
24	12.374	1746	1749	1752	rBV4	6645	7960	1.42%	0.159%
25	12.421	1754	1757	1759	rBV	11896	12029	2.14%	0.240%
26	12.516	1768	1773	1774	rBV5	13956	15411	2.74%	0.307%
27	12.586	1782	1785	1788	rVB	164793	130627	23.26%	2.601%
28	12.763	1813	1815	1817	rVB3	9685	8911	1.59%	0.177%
29	12.816	1817	1824	1828	rBV	147465	163834	29.18%	3.263%
30	12.863	1830	1832	1834	rBV2	6368	7517	1.34%	0.150%
31	12.957	1841	1848	1851	rBV	587899	544781	97.02%	10.849%
32	12.980	1851	1852	1855	rVB3	8778	7118	1.27%	0.142%
33	13.033	1856	1861	1866	rBV8	15181	26827	4.78%	0.534%
34	13.121	1873	1876	1877	rBV3	14455	14362	2.56%	0.286%
35	13.139	1877	1879	1883	rVB4	18774	20271	3.61%	0.404%
36	13.204	1889	1890	1893	rBV3	11645	9797	1.74%	0.195%

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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
 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	13.245	1893	1897	1903	rVV8	23616	36914	6.57%	0.735%
38	13.304	1905	1907	1909	rVB3	14949	12410	2.21%	0.247%
39	13.339	1909	1913	1915	rBV4	21596	26540	4.73%	0.529%
40	13.368	1916	1918	1921	rBV3	16719	13962	2.49%	0.278%
41	13.657	1965	1967	1968	rBV2	19726	15537	2.77%	0.309%
42	13.763	1983	1985	1987	rVB3	17350	9603	1.71%	0.191%
43	13.868	2001	2003	2005	rVB3	16718	10832	1.93%	0.216%
44	14.015	2022	2028	2031	rBV2	253866	310932	55.37%	6.192%
45	14.039	2031	2032	2037	rVB	60260	54677	9.74%	1.089%
46	14.862	2170	2172	2175	rBV4	32347	32713	5.83%	0.651%
47	15.062	2204	2206	2210	rBV4	35577	39830	7.09%	0.793%
48	15.498	2276	2280	2290	rVB	128012	194198	34.58%	3.867%
49	16.986	2529	2533	2534	rBV4	18820	29026	5.17%	0.578%
50	17.974	2698	2701	2709	rVB10	24698	41130	7.32%	0.819%
51	18.309	2757	2758	2760	rBV2	16628	11971	2.13%	0.238%

Sum of corrected areas: 5021690

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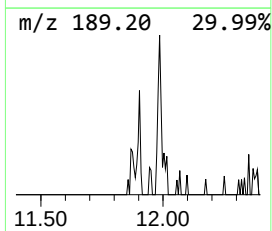
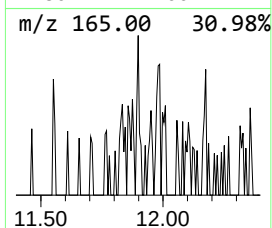
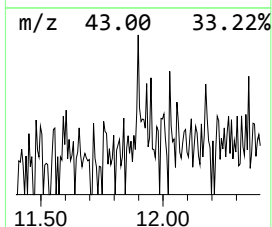
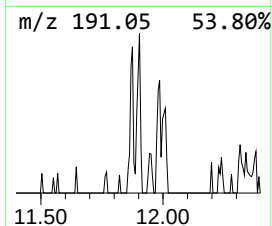
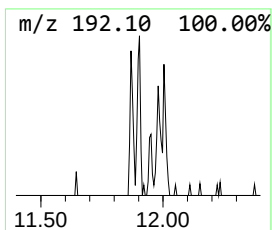
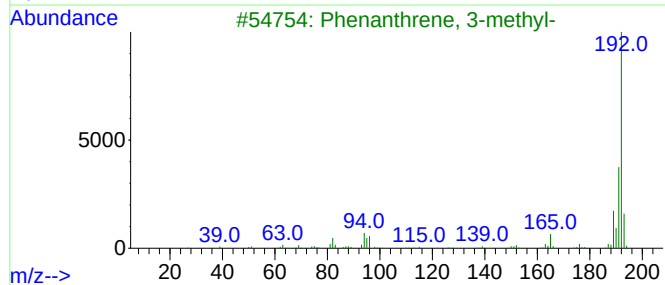
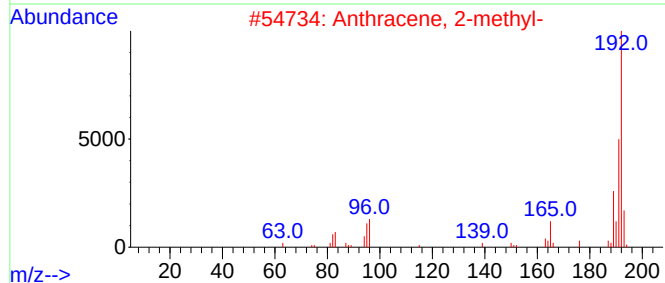
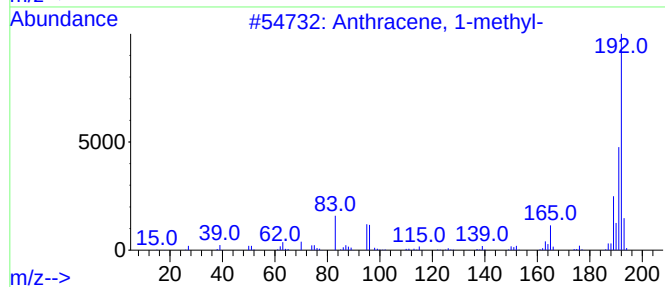
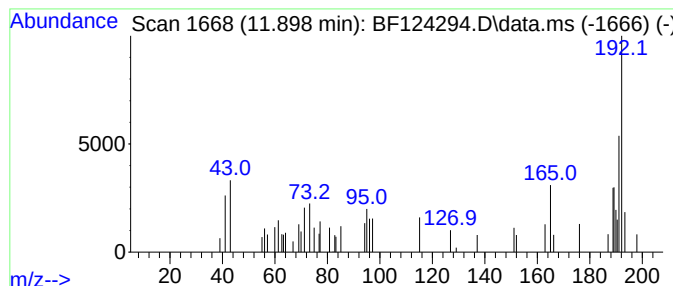
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Anthracene, 1-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	3.11 ng	34805	Phenanthrene-d10	11.369

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Anthracene, 1-methyl-	192	C15H12	000610-48-0	86
2			Anthracene, 2-methyl-	192	C15H12	000613-12-7	70
3			Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	64
4			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	64
5			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	64



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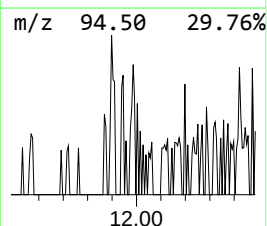
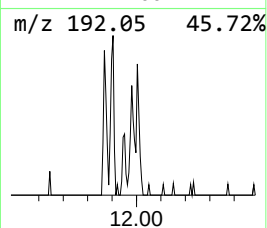
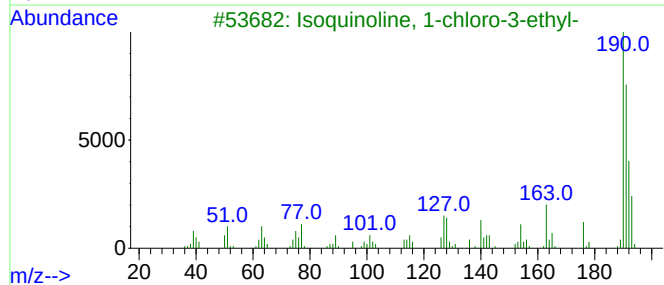
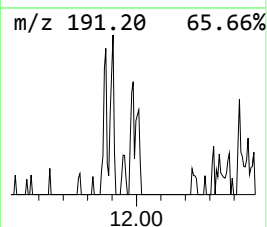
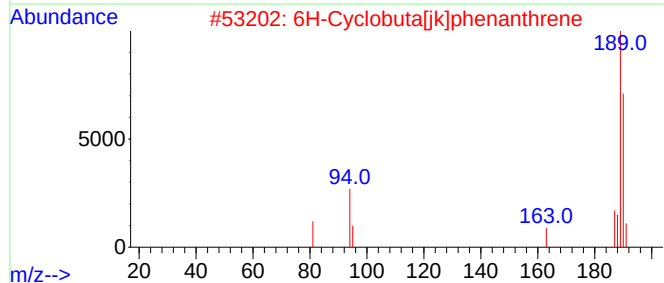
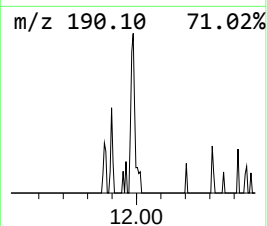
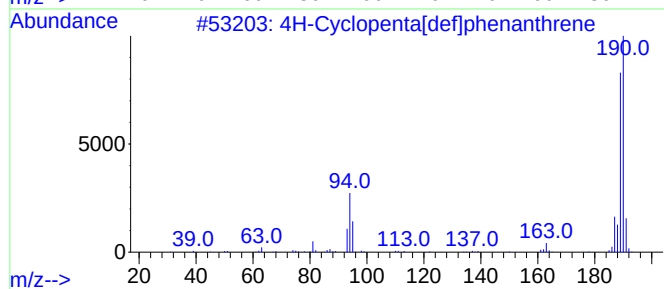
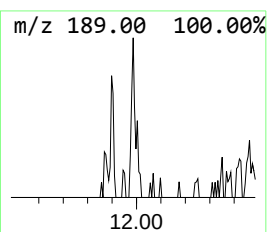
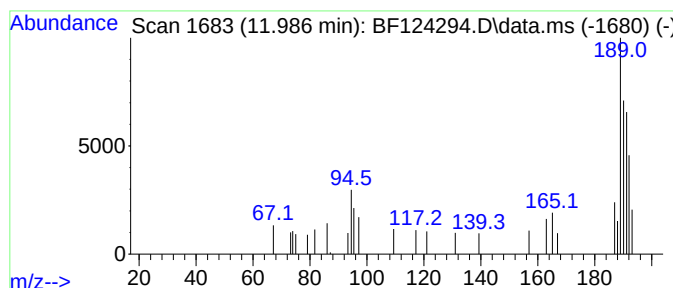
Instrument :
BNA_F
ClientSampled :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.986	2.22 ng	24818	Phenanthrene-d10		11.369	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene		190	C15H10	000203-64-5	58
2	6H-Cyclobuta[jk]phenanthrene		190	C15H10	083469-43-6	49
3	Isoquinoline, 1-chloro-3-ethyl-		191	C11H10ClN	055150-52-2	27
4	1,1'-Biphenyl, 4,4'-difluoro-		190	C12H8F2	000398-23-2	23
5	Methyl diselenide		190	C2H6Se2	007101-31-7	14



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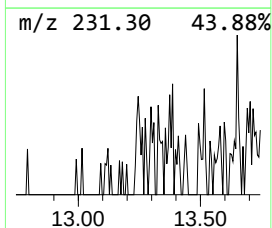
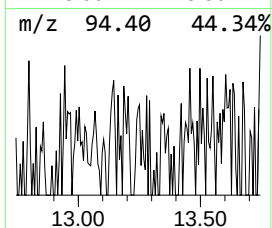
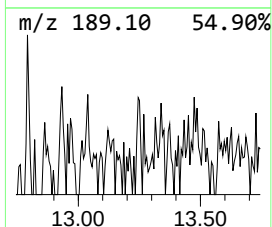
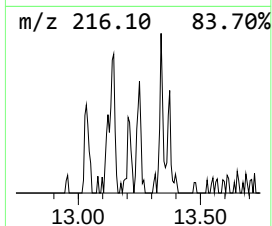
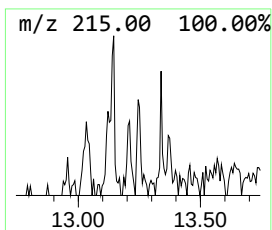
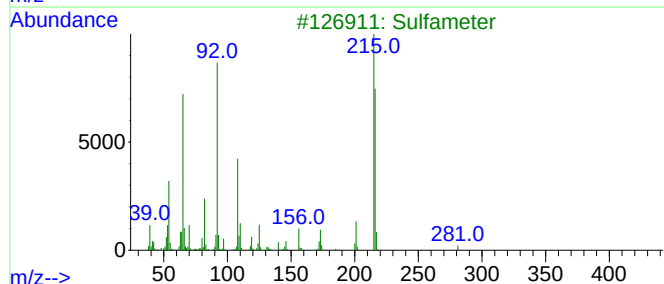
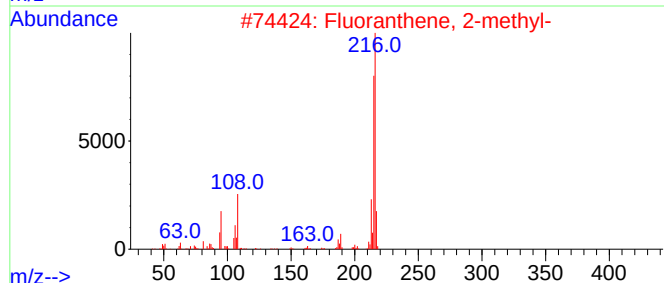
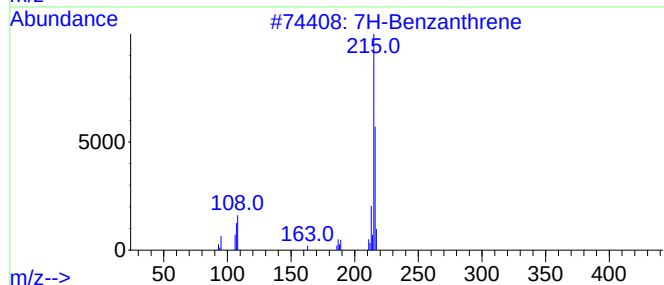
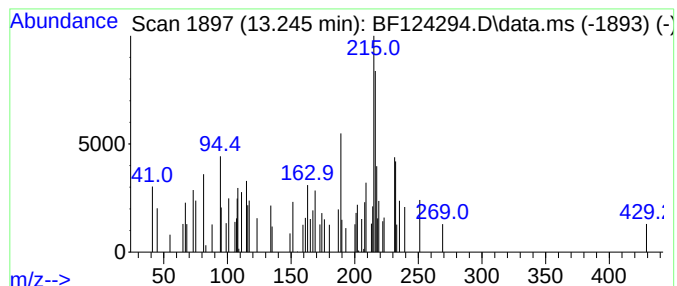
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown13.245 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.245	2.37 ng	36914	Chrysene-d12	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7H-Benzanthrene	216	C17H12	000199-94-0	35
2			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	25
3			Sulfameter	280	C11H12N4O3S	000651-06-9	25
4			3,4-Dichlorocinnamic acid	216	C9H6Cl2O2	001202-39-7	25
5			4-Trifluoromethylcinnamic acid	216	C10H7F3O2	002062-26-2	25



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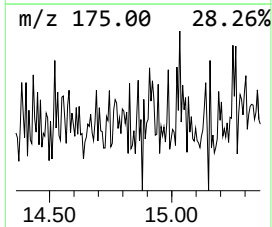
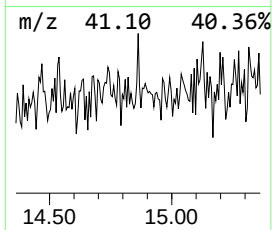
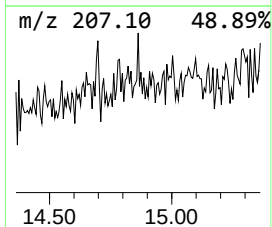
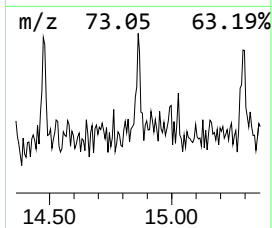
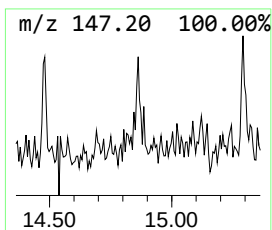
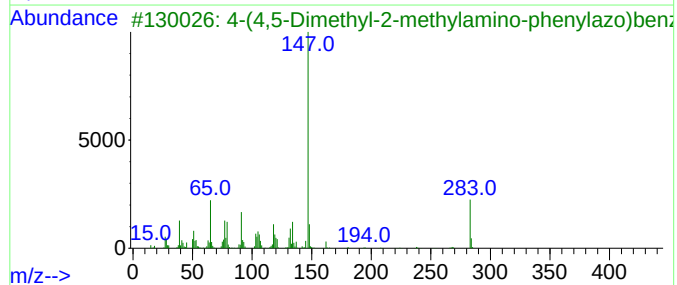
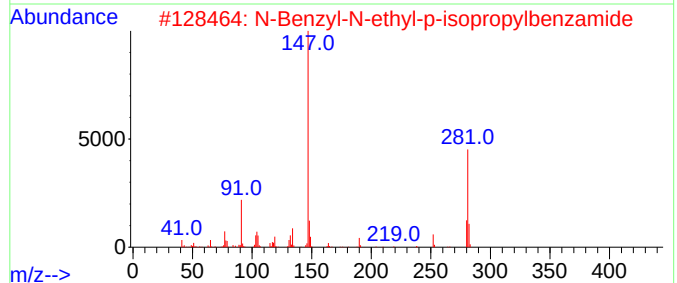
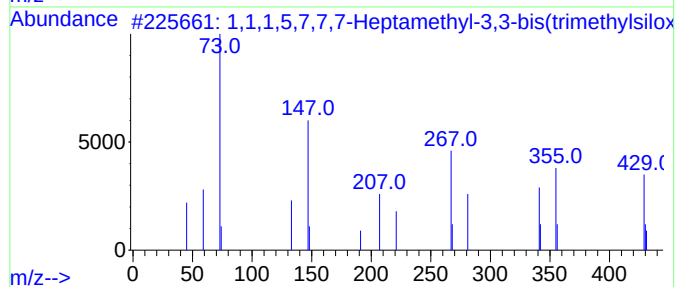
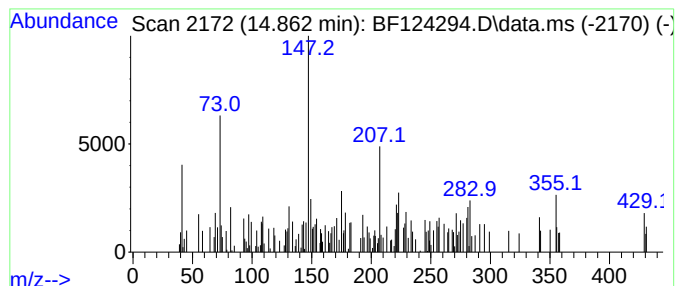
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown14.863 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.863	3.37 ng	32713	Perylene-d12	15.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	35		
2	N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	25		
3	4-(4,5-Dimethyl-2-methylamino-ph...	283	C16H17N3O2	079333-14-5	25		
4	2,3,5,6-Tetramethylbenzyl chloride	182	C11H15Cl	007435-83-8	22		
5	Hexanoic acid, 6-[[4-(1-methylet...	277	C16H23NO3	1000351-17-8	22		



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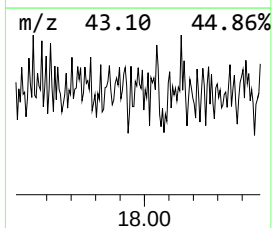
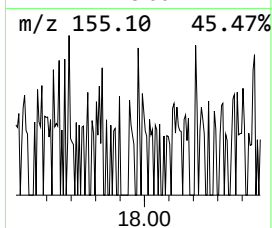
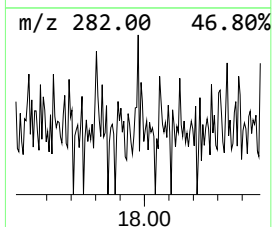
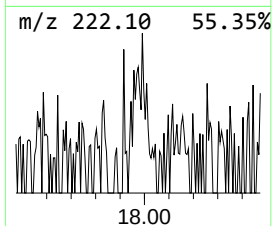
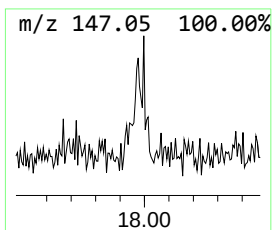
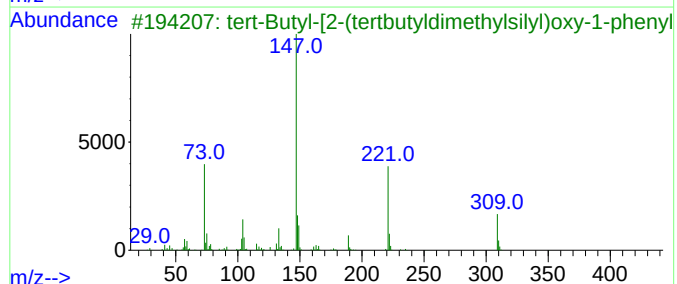
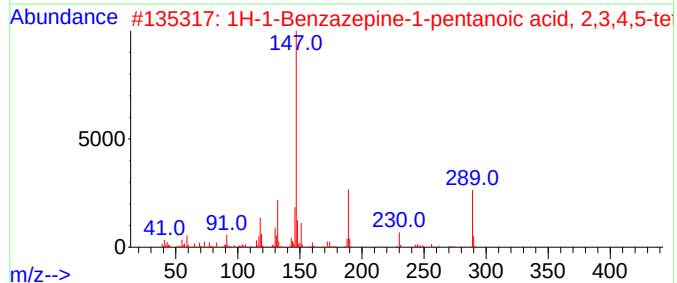
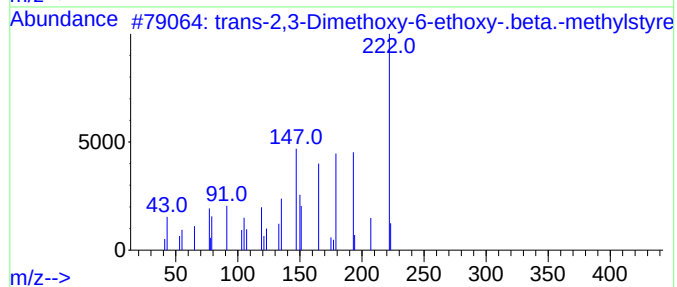
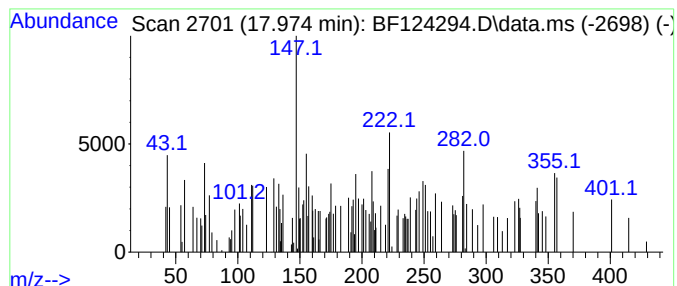
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown17.974 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.974	4.24 ng	41130	Perylene-d12	15.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-2,3-Dimethoxy-6-ethoxy-.be...	222	C13H18O3	1000122-72-4	11
2			1H-1-Benzazepine-1-pentanoic aci...	289	C17H23NO3	1000337-77-9	10
3			tert-Butyl-[2-(tertbutyldimethyl...	366	C20H38O2Si2	1000373-40-4	10
4			1,3-Benzenediol, 0,0'-dipropargy...	274	C14H10O6	1000345-53-0	10
5			Tetrazole, 1-(2-fluorophenyl)-5-...	342	C18H19FN4S	1000272-52-4	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061221\
Data File : BF124294.D
Acq On : 12 Jun 2021 19:23
Operator : JU/CG
Sample : M2639-01 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B67

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
Anthracene, 1-m...	11.898	3.1	ng	34805	4	11.369	223638	20.0
4H-Cyclopenta[d...	11.986	2.2	ng	24818	4	11.369	223638	20.0
unknown13.245	13.245	2.4	ng	36914	5	14.015	310932	20.0
unknown14.863	14.863	3.4	ng	32713	6	15.498	194198	20.0
unknown17.974	17.974	4.2	ng	41130	6	15.498	194198	20.0