

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102620\
 Data File : BF122122.D
 Acq On : 26 Oct 2020 18:40
 Operator : JU/CG
 Sample : L4510-17
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-2

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-BF101220.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122122.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.334	549	552	580	rBV	1683465	1924636	85.13%	9.896%
2	6.363	724	727	755	rBV	1937895	1969863	87.13%	10.129%
3	6.710	783	786	798	rVB	624022	578595	25.59%	2.975%
4	7.281	879	883	897	rBV	1389147	1350605	59.74%	6.945%
5	7.992	1001	1004	1008	rBV	758596	778162	34.42%	4.001%
6	9.069	1183	1187	1190	rBV	2652125	2260883	100.00%	11.625%
7	9.469	1252	1255	1263	rBV	216098	179445	7.94%	0.923%
8	9.745	1298	1302	1305	rBV	1053999	872432	38.59%	4.486%
9	9.781	1305	1308	1315	rVB	97964	95531	4.23%	0.491%
10	9.957	1334	1338	1342	rBV	32873	29594	1.31%	0.152%
11	10.298	1392	1396	1402	rBV	62557	58798	2.60%	0.302%
12	10.539	1433	1437	1447	rBV	1204782	1195784	52.89%	6.149%
13	11.233	1551	1555	1557	rBV	981354	918702	40.63%	4.724%
14	11.257	1557	1559	1563	rVV	453283	372019	16.45%	1.913%
15	11.310	1563	1568	1573	rVB	128458	122922	5.44%	0.632%
16	11.475	1592	1596	1602	rBV2	48832	48851	2.16%	0.251%
17	11.733	1637	1640	1643	rBV	30800	28718	1.27%	0.148%
18	11.763	1643	1645	1651	rVB2	55081	54927	2.43%	0.282%
19	11.845	1656	1659	1662	rBV	68833	66279	2.93%	0.341%
20	12.445	1758	1761	1765	rBV	455590	388608	17.19%	1.998%
21	12.545	1774	1778	1784	rBV2	21006	35586	1.57%	0.183%
22	12.674	1795	1800	1807	rVB	355312	387656	17.15%	1.993%
23	12.816	1819	1824	1827	rBV	2514195	2155059	95.32%	11.081%
24	12.898	1833	1838	1842	rVB2	18008	28279	1.25%	0.145%
25	13.004	1853	1856	1859	rVB	53208	47891	2.12%	0.246%
26	13.069	1864	1867	1870	rVB	56463	47837	2.12%	0.246%
27	13.110	1870	1874	1875	rBV2	24835	27569	1.22%	0.142%
28	13.292	1900	1905	1914	rBV	729046	787906	34.85%	4.051%
29	13.627	1957	1962	1964	rBV	24668	31967	1.41%	0.164%
30	13.727	1972	1979	1987	rVB6	97076	224203	9.92%	1.153%
31	13.874	1996	2004	2007	rBV2	781590	887548	39.26%	4.564%
32	13.898	2007	2008	2011	rVB	146512	97653	4.32%	0.502%
33	13.980	2019	2022	2025	rVB	38271	34644	1.53%	0.178%
34	14.263	2066	2070	2073	rBV	30808	38606	1.71%	0.199%
35	14.627	2129	2132	2137	rVB	27528	33386	1.48%	0.172%
36	14.898	2174	2178	2181	rBV	119192	160879	7.12%	0.827%

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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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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-BF101220.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.004	2193	2196	2201	rVB	22877	27663	1.22%	0.142%
38	15.186	2224	2227	2233	rVB	73462	80329	3.55%	0.413%
39	15.245	2233	2237	2242	rBV	105612	116744	5.16%	0.600%
40	15.304	2242	2247	2259	rVB	544120	682657	30.19%	3.510%
41	15.698	2310	2314	2319	rBV2	22918	34624	1.53%	0.178%
42	16.710	2480	2486	2491	rBV	53287	107019	4.73%	0.550%
43	17.133	2554	2558	2568	rVB2	36388	76649	3.39%	0.394%

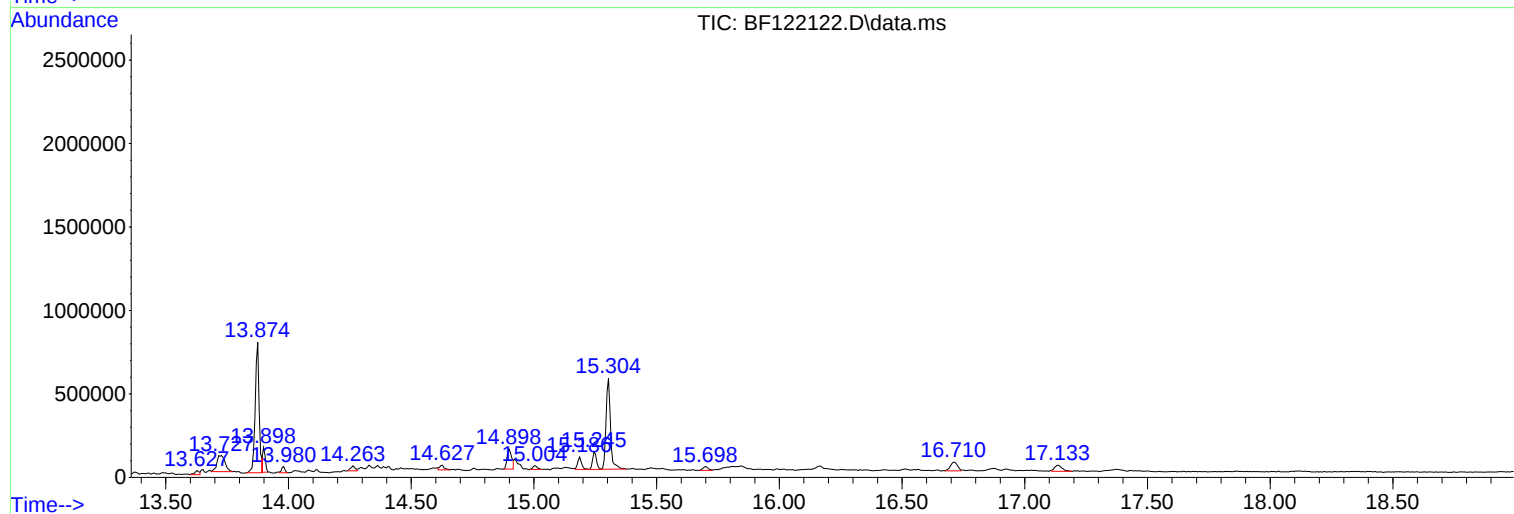
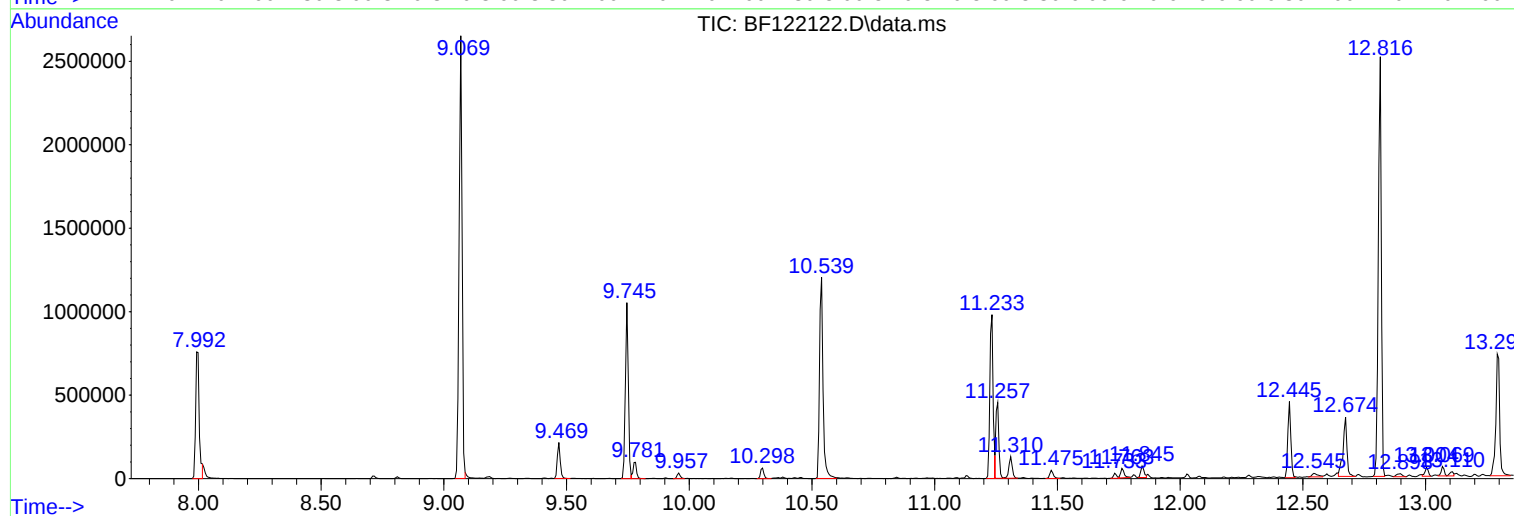
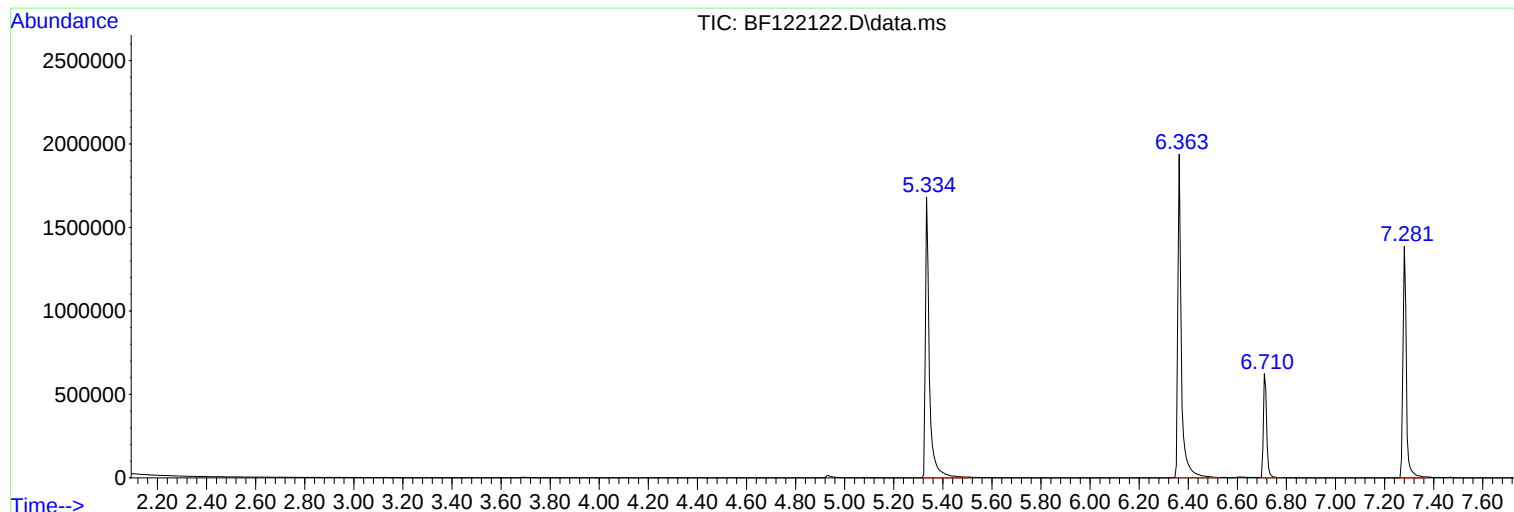
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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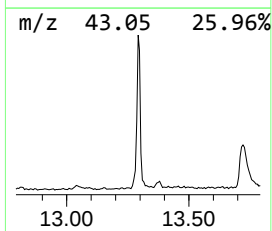
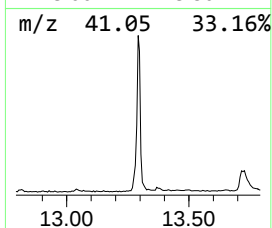
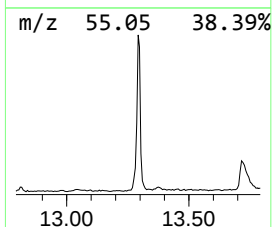
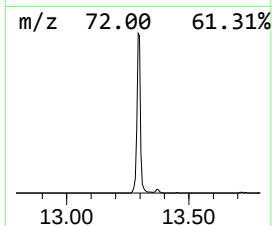
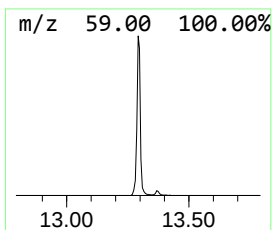
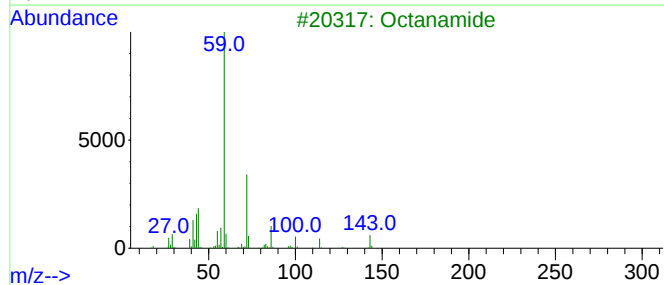
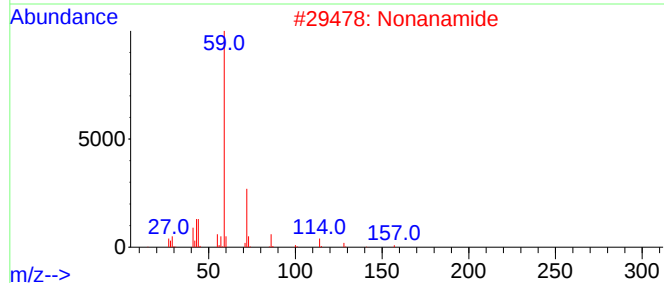
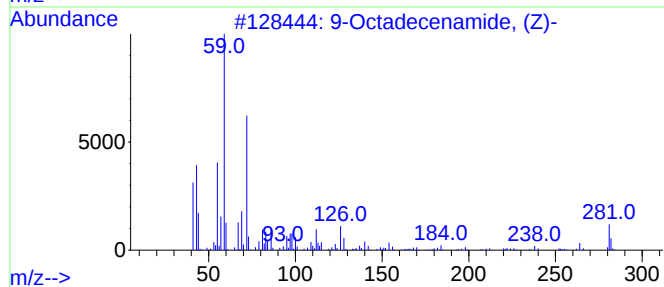
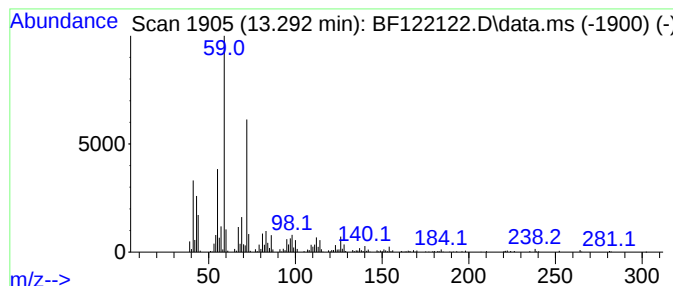
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 9-Octadecenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	17.75 ng	787906	Chrysene-d12	13.874

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	95
2			Nonanamide	157	C9H19NO	001120-07-6	59
3			Octanamide	143	C8H17NO	000629-01-6	53
4			Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	50
5			Dodecanamide	199	C12H25NO	001120-16-7	45



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Instrument :
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ClientSampleId :
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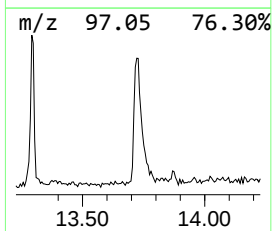
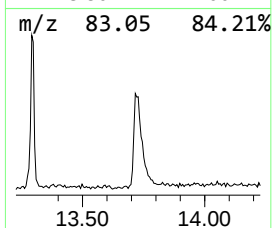
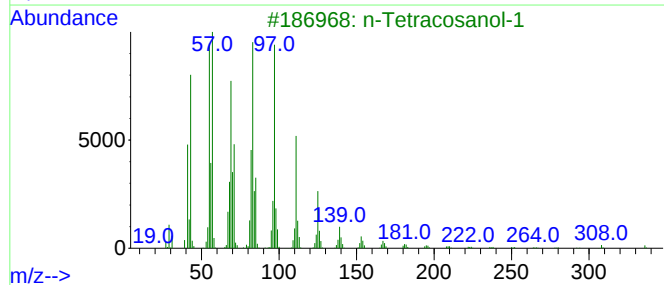
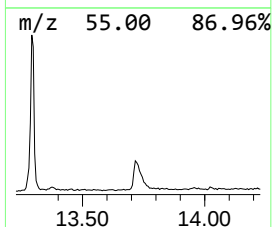
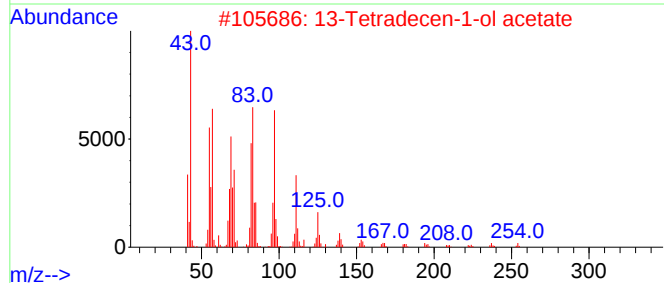
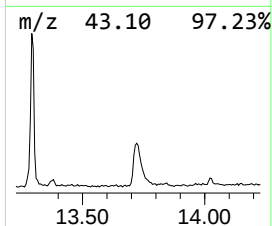
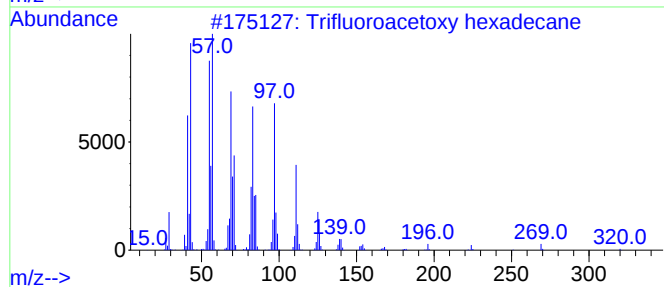
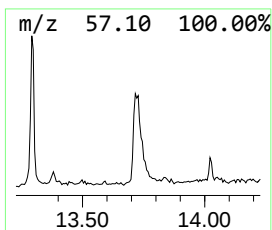
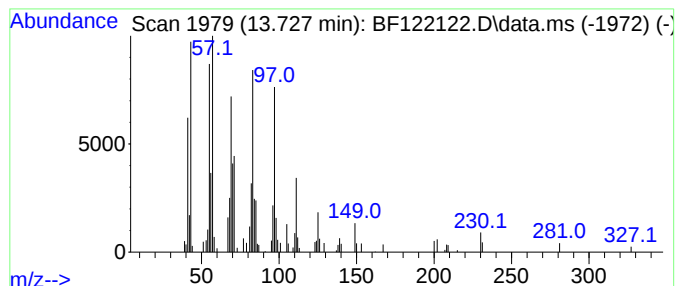
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Trifluoroacetoxy hexadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.727	5.05 ng	224203	Chrysene-d12	13.874

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90
2			13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	87
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	87
4			Octacosanol	410	C28H58O	000557-61-9	87
5			1-Docosene	308	C22H44	001599-67-3	81



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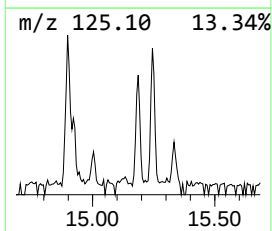
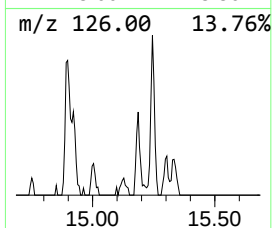
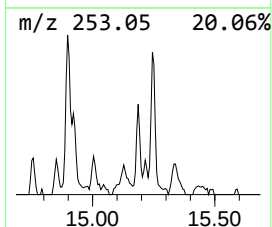
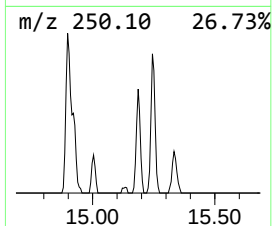
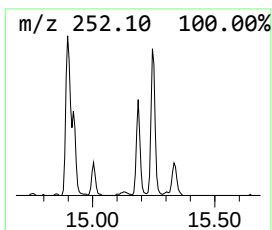
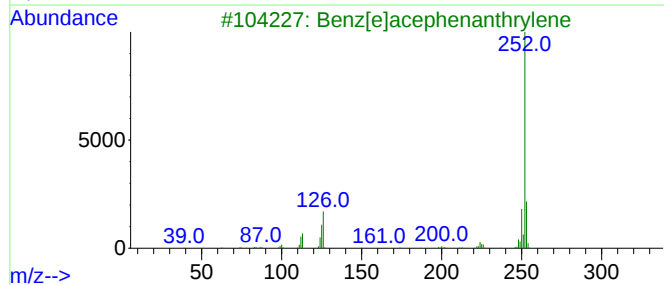
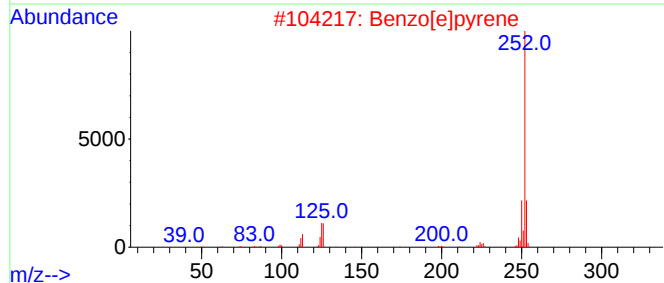
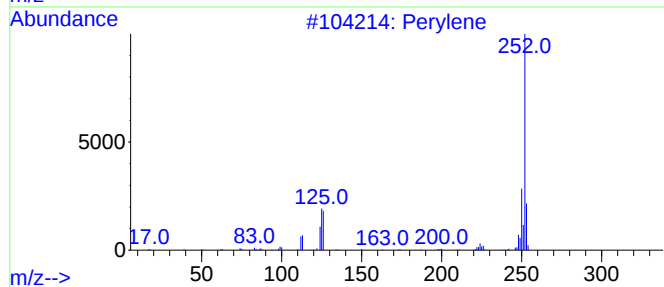
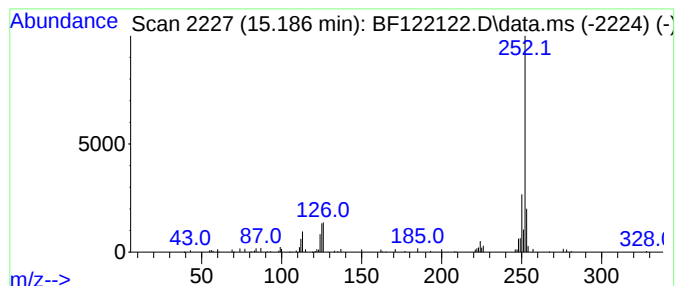
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Perylene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.186	2.35 ng	80329	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Perylene	252	C20H12	000198-55-0	98
2			Benzo[e]pyrene	252	C20H12	000192-97-2	96
3			Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	95
4			Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
5			Benzo[a]pyrene	252	C20H12	000050-32-8	91



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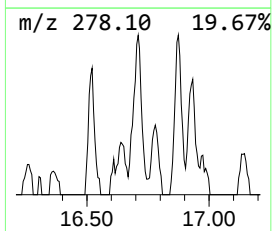
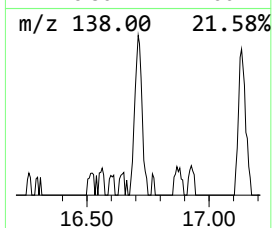
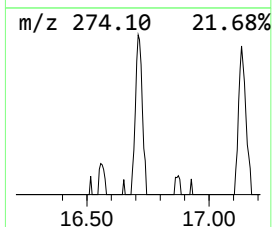
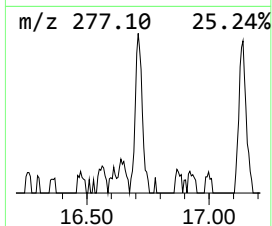
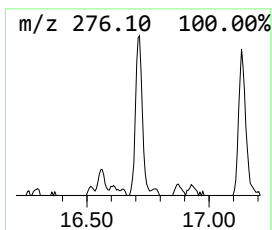
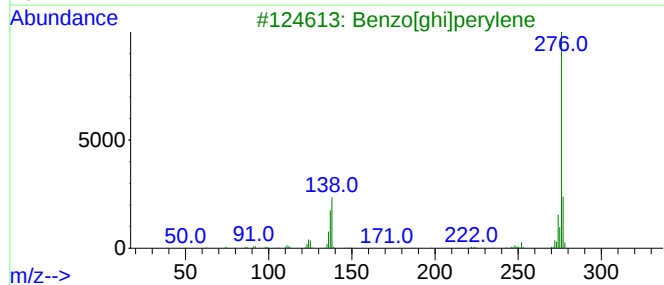
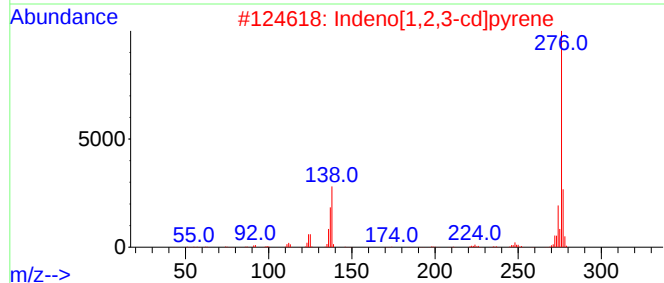
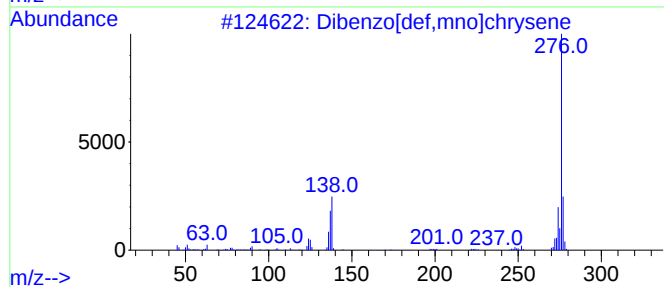
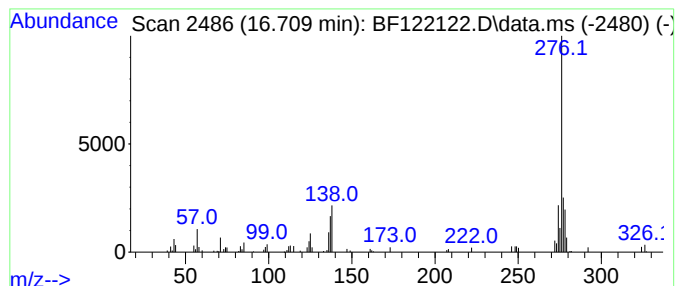
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Dibenzo[def,mno]chrysene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.709	3.14 ng	107019	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	93
2			Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	89
3			Benzo[ghi]perylene	276	C22H12	000191-24-2	89
4			Indeno[1,2,3-cd]fluoranthene	276	C22H12	000193-43-1	86
5			2-Thiophenecarbaldehyde, 5-[5-(t...	276	C13H8OS3	1000217-28-5	40



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
9-Octadecenamid...	13.292	17.8	ng	787906	5	13.874	887548	20.0
Trifluoroacetox...	13.727	5.0	ng	224203	5	13.874	887548	20.0
Perylene	15.186	2.4	ng	80329	6	15.304	682657	20.0
Dibenzo[def,mno...	16.709	3.1	ng	107019	6	15.304	682657	20.0