

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072723\
 Data File : BF134507.D
 Acq On : 27 Jul 2023 15:56
 Operator : CG\JU
 Sample : 03736-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TR-5-072423

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-BF072423.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134507.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.457	570	573	588	rBV	907053	921179	61.23%	6.594%
2	6.463	741	744	762	rBV	1505678	1504464	100.00%	10.770%
3	6.822	802	805	824	rVB	767325	650369	43.23%	4.656%
4	7.387	897	901	912	rBV	1038754	931580	61.92%	6.669%
5	7.463	912	914	927	rVB8	10239	22338	1.48%	0.160%
6	8.098	1019	1022	1036	rVB	921340	877811	58.35%	6.284%
7	8.816	1142	1144	1146	rBV	18841	15149	1.01%	0.108%
8	8.916	1156	1161	1164	rBV	19305	20609	1.37%	0.148%
9	9.175	1201	1205	1209	rBV	1472570	1250087	83.09%	8.949%
10	9.445	1244	1251	1256	rBV8	8447	15273	1.02%	0.109%
11	9.575	1270	1273	1280	rVB	85143	69731	4.63%	0.499%
12	9.857	1318	1321	1324	rBV	654970	522213	34.71%	3.738%
13	9.892	1324	1327	1330	rVB	73271	61466	4.09%	0.440%
14	10.063	1353	1356	1361	rBV	40324	39033	2.59%	0.279%
15	10.286	1391	1394	1396	rVB2	17931	16335	1.09%	0.117%
16	10.410	1412	1415	1421	rVB	65034	55989	3.72%	0.401%
17	10.651	1452	1456	1467	rBV	777956	667047	44.34%	4.775%
18	10.763	1472	1475	1484	rVB5	21530	38674	2.57%	0.277%
19	10.957	1505	1508	1511	rBV5	11449	16555	1.10%	0.119%
20	11.210	1547	1551	1554	rBV3	36174	33226	2.21%	0.238%
21	11.251	1554	1558	1563	rVB2	30916	43188	2.87%	0.309%
22	11.304	1563	1567	1572	rBV5	10291	16433	1.09%	0.118%
23	11.351	1572	1575	1577	rVV	568873	494950	32.90%	3.543%
24	11.375	1577	1579	1583	rVV	409551	359598	23.90%	2.574%
25	11.428	1585	1588	1591	rVV	93516	85642	5.69%	0.613%
26	11.457	1591	1593	1600	rVB7	13245	22088	1.47%	0.158%
27	11.592	1613	1616	1621	rVB	50587	45645	3.03%	0.327%
28	11.639	1621	1624	1629	rVB2	21821	24044	1.60%	0.172%
29	11.857	1658	1661	1662	rBV	34321	30985	2.06%	0.222%
30	11.880	1662	1665	1672	rVB2	296431	292102	19.42%	2.091%
31	11.969	1677	1680	1683	rVV	81183	81228	5.40%	0.581%
32	11.992	1683	1684	1688	rVB	25311	16023	1.07%	0.115%
33	12.151	1708	1711	1714	rBV	29357	31268	2.08%	0.224%
34	12.186	1714	1717	1721	rVB2	29314	31956	2.12%	0.229%
35	12.304	1731	1737	1739	rBV8	12888	22641	1.50%	0.162%
36	12.410	1752	1755	1757	rBV2	28074	33982	2.26%	0.243%

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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

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37	12.433	1757	1759	1767	rVB5	52327	91798	6.10%	0.657%
38	12.504	1767	1771	1774	rBV2	19351	25034	1.66%	0.179%
39	12.575	1779	1783	1787	rBV	630740	534926	35.56%	3.829%
40	12.669	1796	1799	1804	rBV	113524	120015	7.98%	0.859%
41	12.727	1806	1809	1811	rVB2	23800	25474	1.69%	0.182%
42	12.804	1816	1822	1828	rBV	467630	532555	35.40%	3.812%
43	12.857	1829	1831	1835	rVB2	27781	27868	1.85%	0.200%
44	12.945	1840	1846	1849	rBV	1284398	1114546	74.08%	7.979%
45	13.022	1855	1859	1864	rBV3	27714	53960	3.59%	0.386%
46	13.133	1876	1878	1881	rVB	67416	58641	3.90%	0.420%
47	13.175	1882	1885	1887	rBV2	28676	32746	2.18%	0.234%
48	13.204	1887	1890	1892	rVB	57280	50143	3.33%	0.359%
49	13.239	1893	1896	1898	rBV3	33979	38976	2.59%	0.279%
50	13.363	1915	1917	1919	rBV2	22837	20722	1.38%	0.148%
51	13.516	1940	1943	1946	rBV2	41842	42101	2.80%	0.301%
52	13.757	1982	1984	1987	rBV	34966	31216	2.07%	0.223%
53	13.810	1991	1993	1997	rVV2	30822	42819	2.85%	0.307%
54	13.863	1997	2002	2008	rVB5	67773	145599	9.68%	1.042%
55	14.010	2023	2027	2030	rBV2	491193	583335	38.77%	4.176%
56	14.039	2030	2032	2036	rVB	165494	136026	9.04%	0.974%
57	14.116	2043	2045	2048	rBV	35239	29811	1.98%	0.213%
58	15.074	2204	2208	2211	rBV	114723	169651	11.28%	1.214%
59	15.380	2258	2260	2264	rVB	64410	62967	4.19%	0.451%
60	15.445	2268	2271	2277	rVB	109185	148619	9.88%	1.064%
61	15.510	2278	2282	2286	rBV	242549	322665	21.45%	2.310%
62	16.210	2397	2401	2409	rVB3	88230	165803	11.02%	1.187%

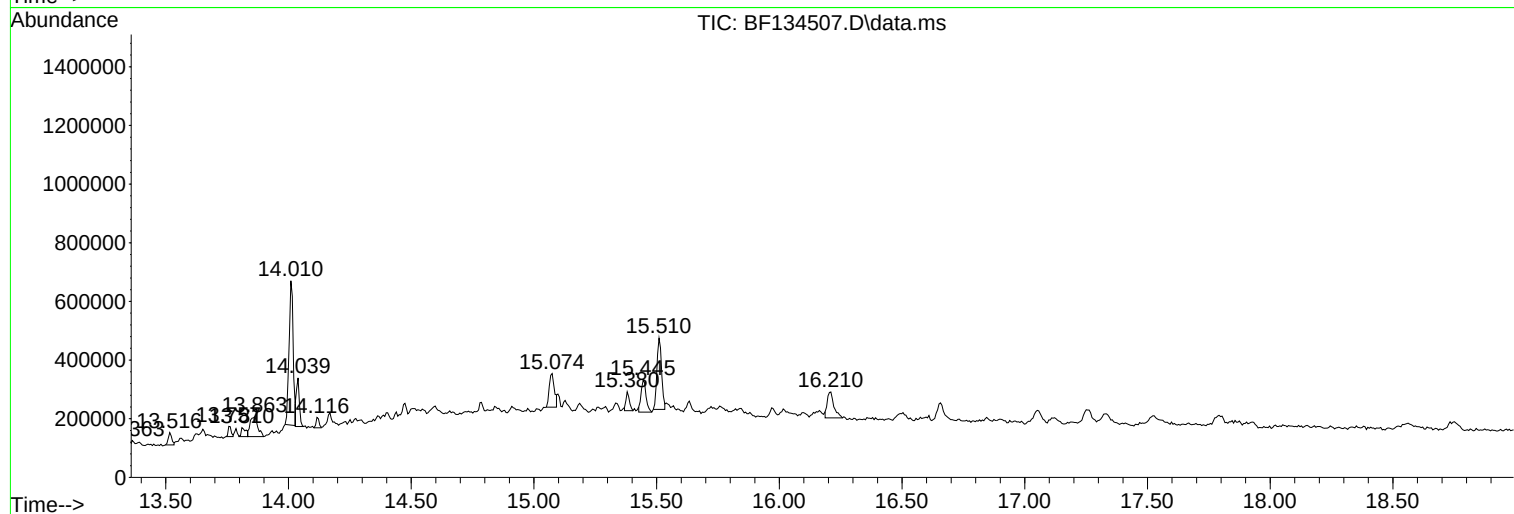
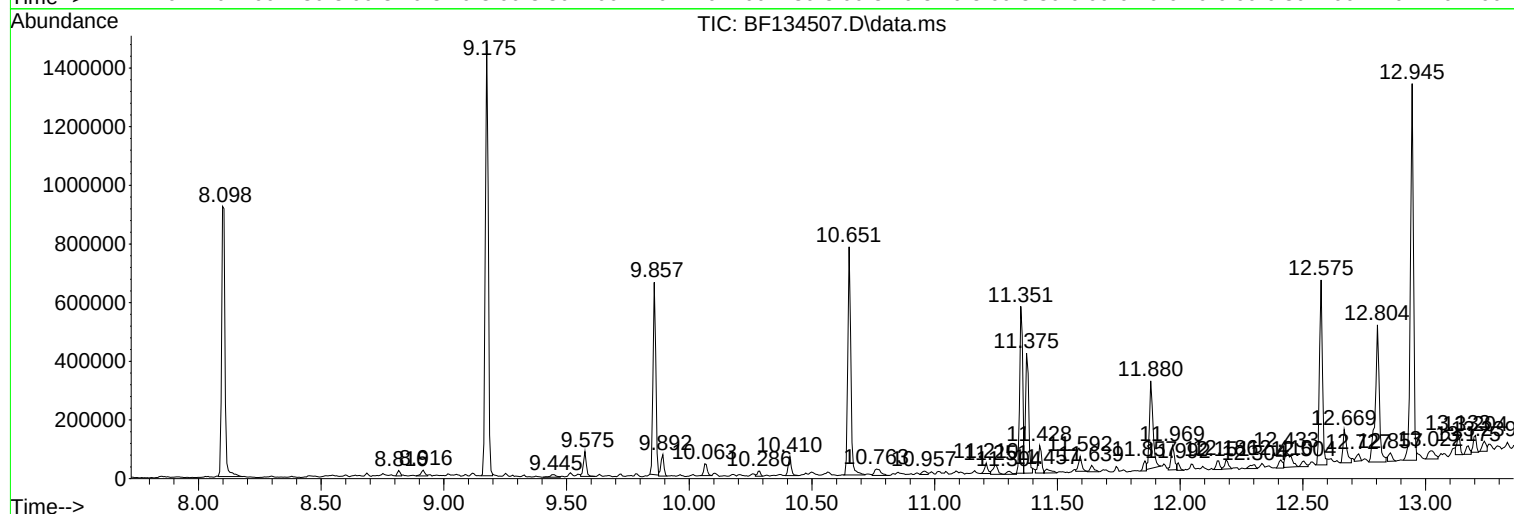
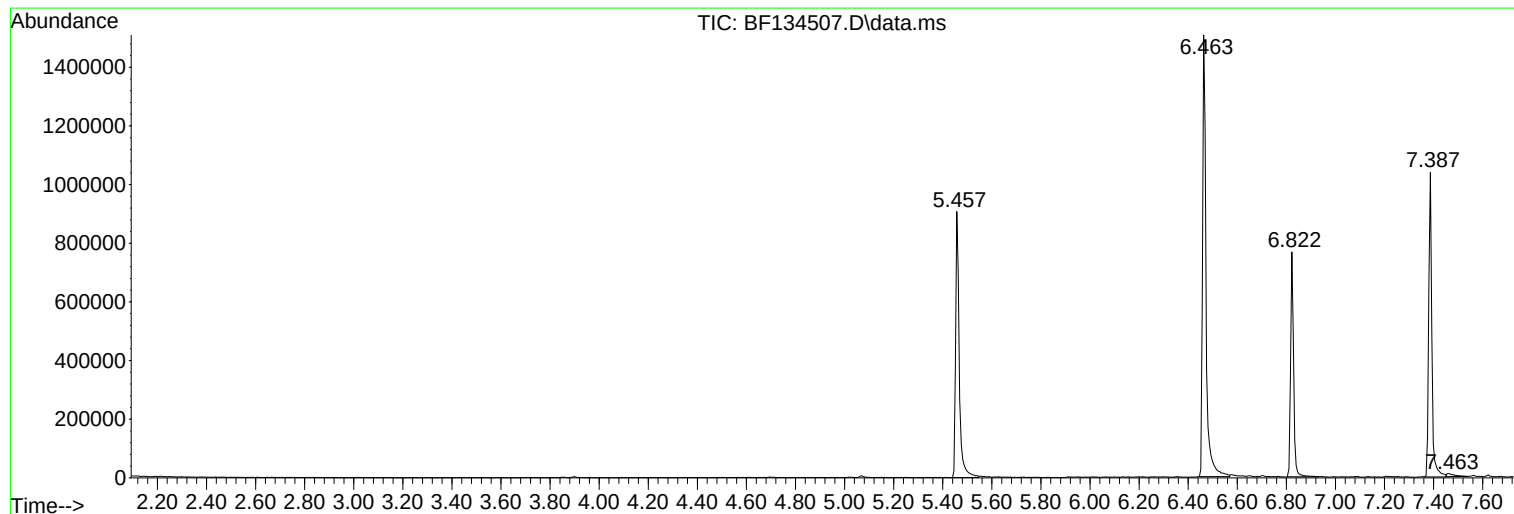
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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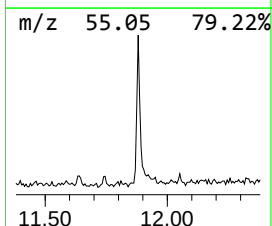
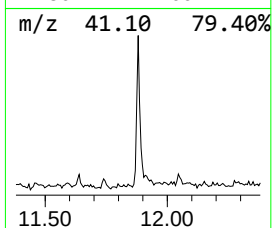
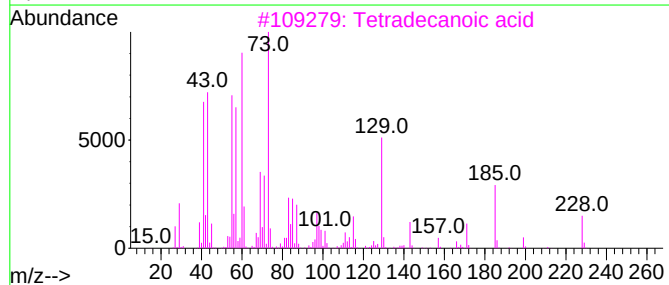
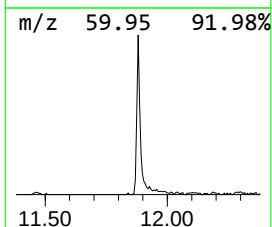
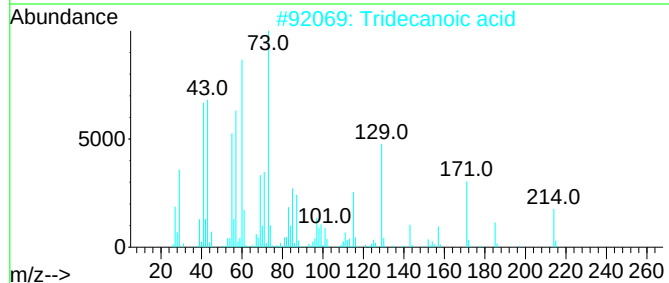
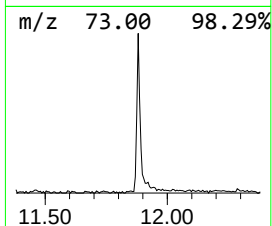
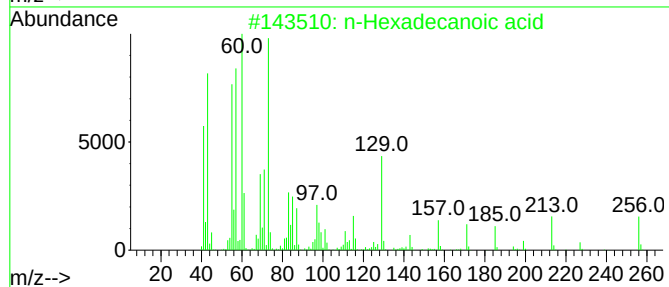
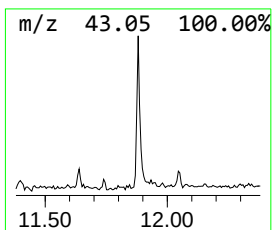
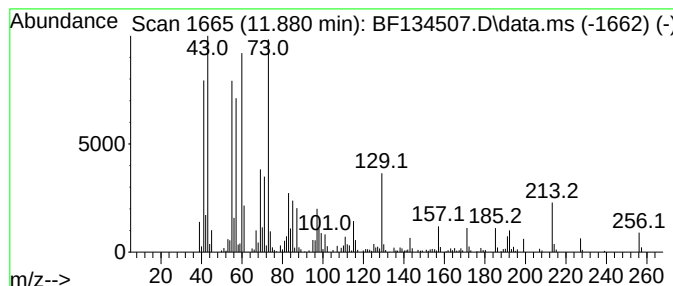
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.881	11.80 ng	292102	Phenanthrene-d10	11.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	96
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	95
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5			n-Decanoic acid	172	C10H20O2	000334-48-5	58



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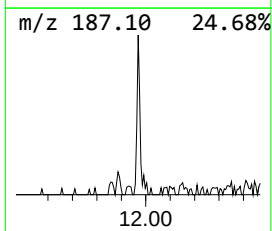
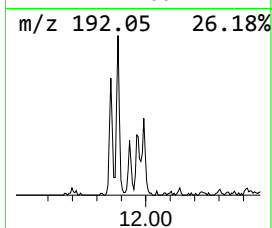
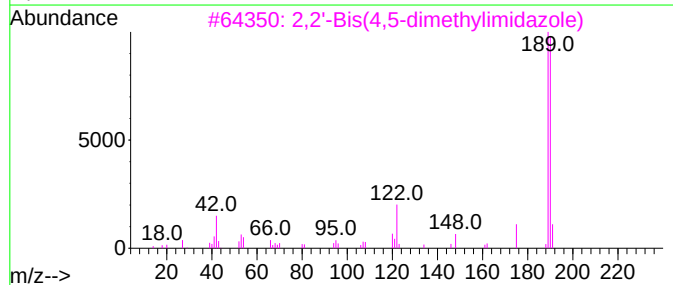
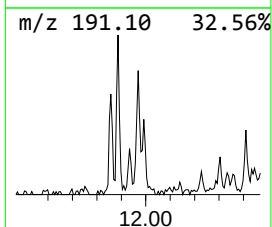
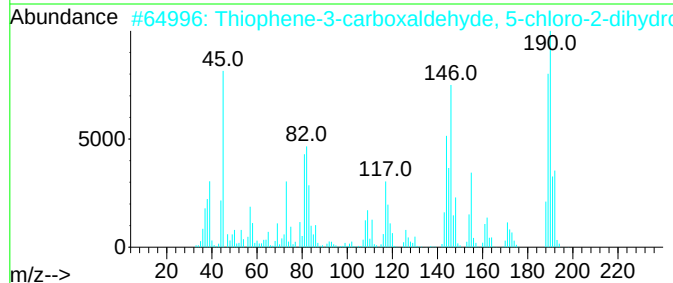
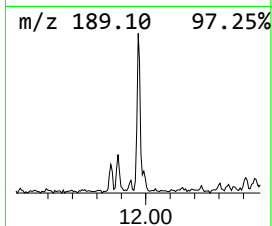
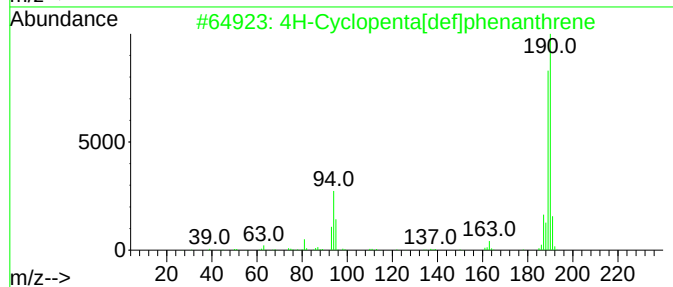
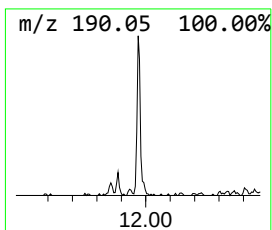
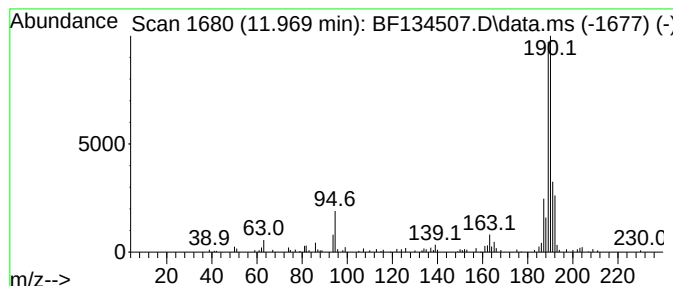
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.969	3.28 ng	81228	Phenanthrene-d10	11.351	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	83
2	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	52
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	50
4	Megastigmatrienone	190	C13H18O	038818-55-2	22
5	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	20



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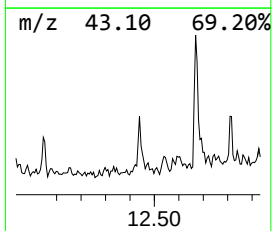
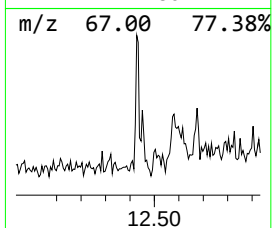
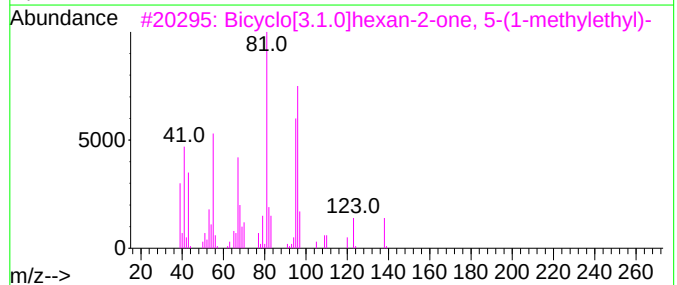
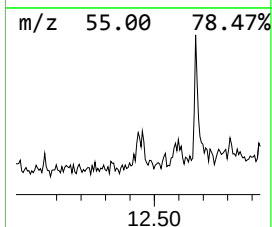
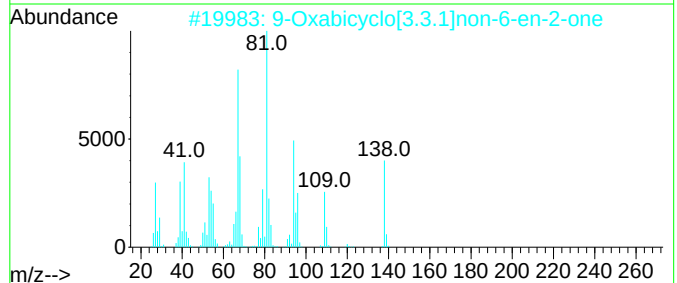
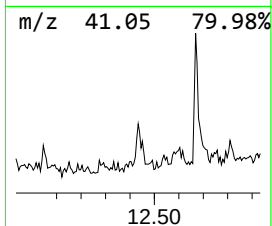
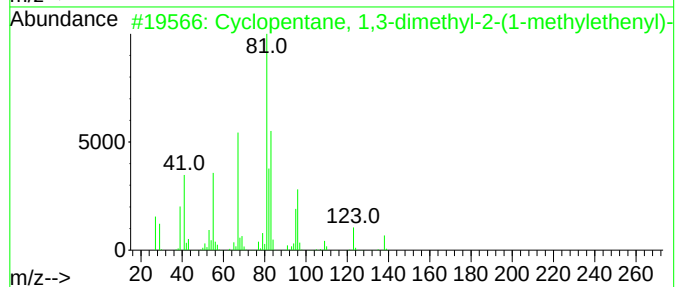
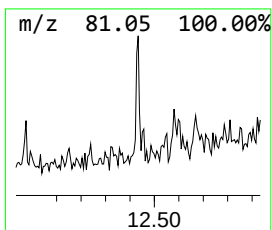
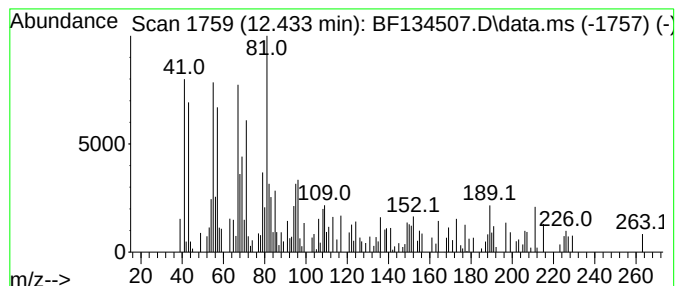
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Cyclopentane, 1,3-dimethyl-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.433	3.71 ng	91798	Phenanthrene-d10	11.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1,3-dimethyl-2-(1-...	138	C10H18	061142-31-2	52
2			9-Oxabicyclo[3.3.1]non-6-en-2-one	138	C8H10O2	1000190-61-5	52
3			Bicyclo[3.1.0]hexan-2-one, 5-(1-...	138	C9H14O	000513-20-2	52
4			1,E-8,Z-10-Pentadecatatriene	206	C15H26	080625-32-7	51
5			1-Isopropylcyclohex-1-ene	124	C9H16	004292-04-0	49



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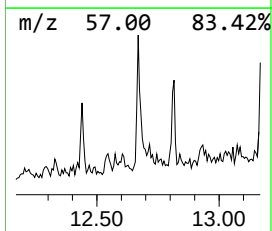
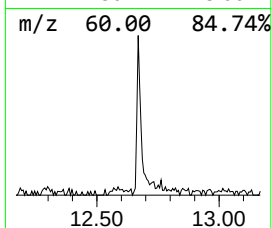
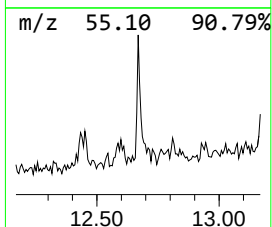
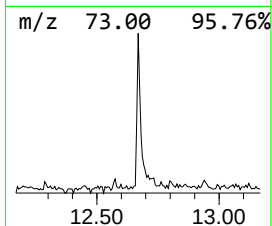
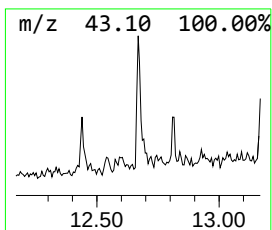
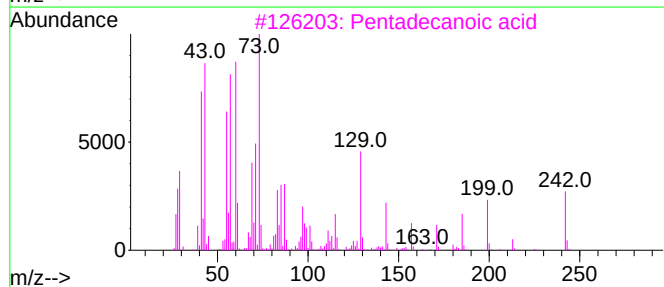
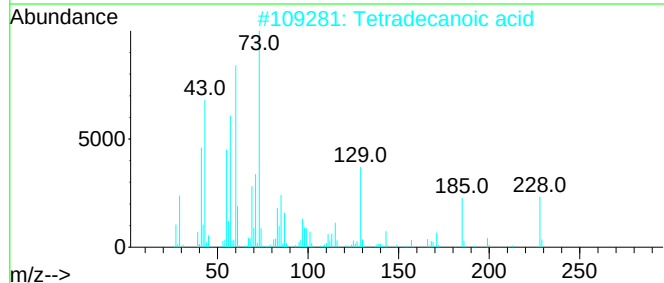
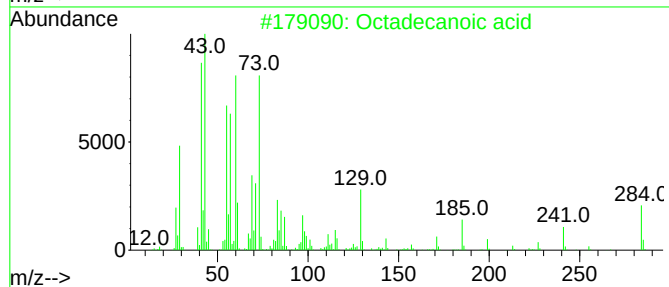
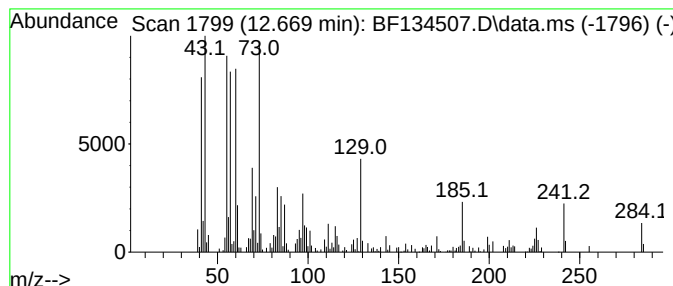
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.669	4.85 ng	120015	Phenanthrene-d10	11.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	93
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
5			Tridecanoic acid	214	C13H26O2	000638-53-9	72



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ClientSampleId :
TR-5-072423

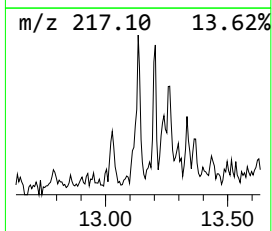
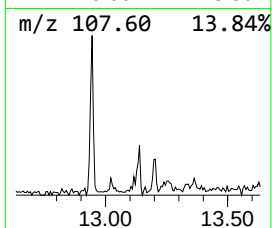
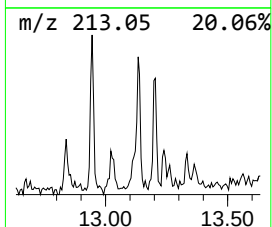
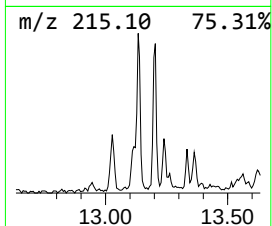
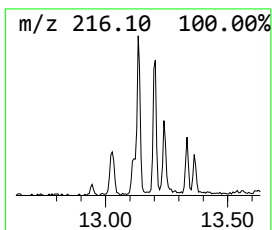
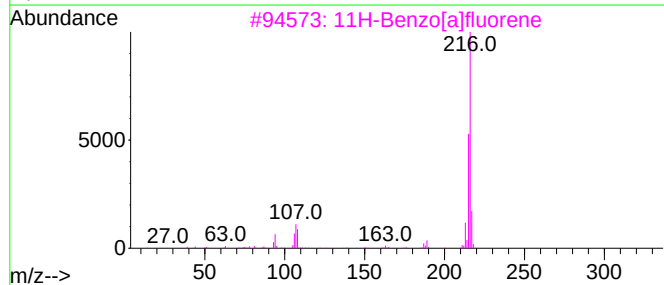
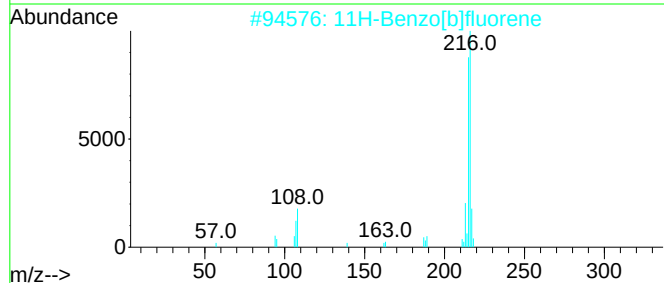
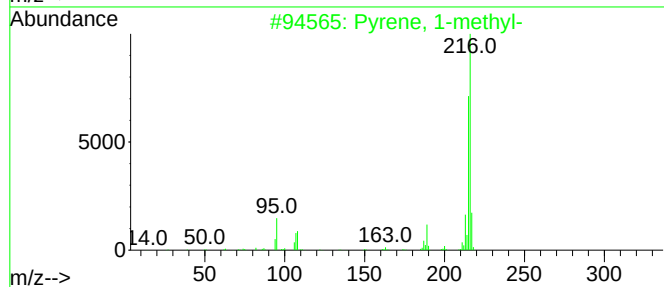
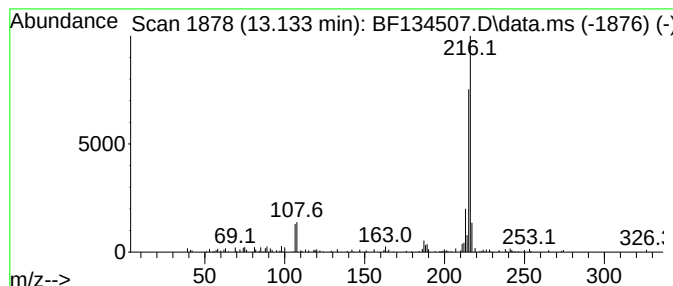
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pyrene, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.133	2.01 ng	58641	Chrysene-d12		14.016

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pyrene, 1-methyl-	216	C17H12	002381-21-7	90
2		11H-Benzo[b]fluorene	216	C17H12	000243-17-4	87
3		11H-Benzo[a]fluorene	216	C17H12	000238-84-6	86
4		Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	74
5		Pyrene, 2-methyl-	216	C17H12	003442-78-2	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072723\
Data File : BF134507.D
Acq On : 27 Jul 2023 15:56
Operator : CG\JU
Sample : 03736-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

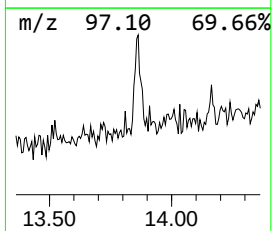
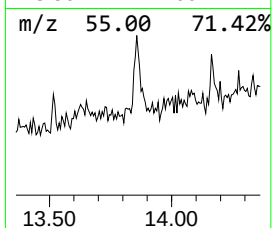
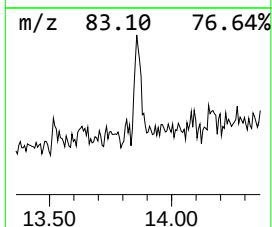
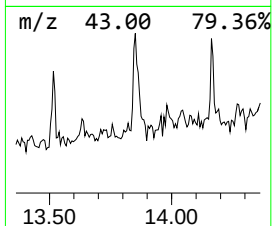
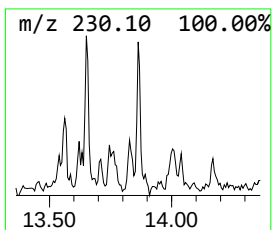
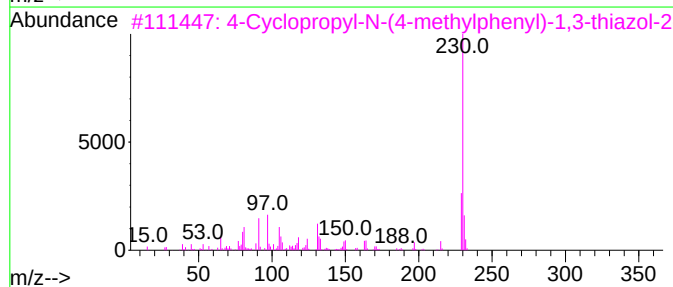
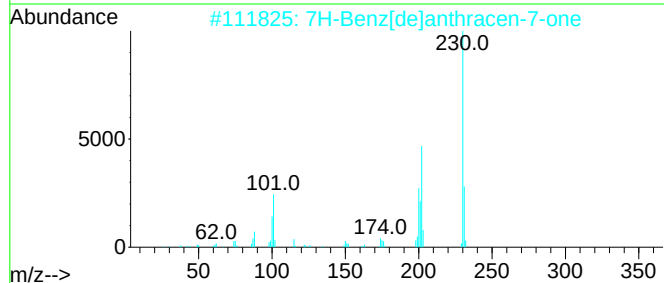
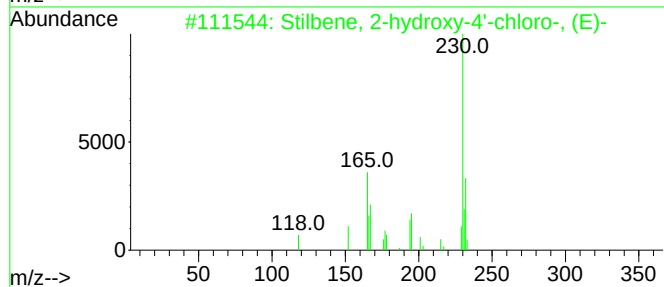
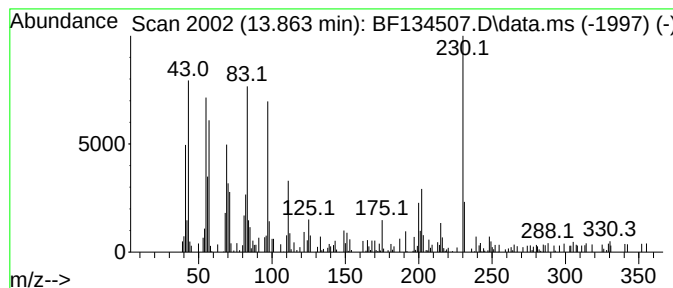
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ClientSampleId :
TR-5-072423

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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 Stilbene, 2-hydroxy-4'-chlo... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.863	4.99 ng	145599	Chrysene-d12	14.016	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Stilbene, 2-hydroxy-4'-chloro-, ...	230	C14H11ClO	1000138-48-2	50
2	7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	41
3	4-Cyclopropyl-N-(4-methylphenyl)...	230	C13H14N2S	1000461-00-1	35
4	Benzene, 1-phenyl-4-(2,2-dicyano...	230	C16H10N2	026089-09-8	25
5	m-Terphenyl	230	C18H14	000092-06-8	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072723\
Data File : BF134507.D
Acq On : 27 Jul 2023 15:56
Operator : CG\JU
Sample : 03736-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-5-072423

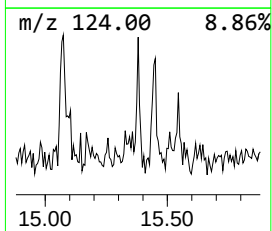
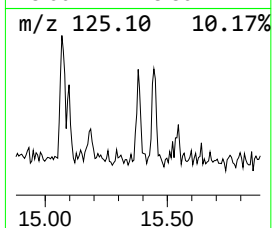
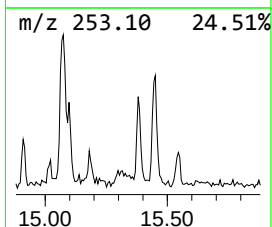
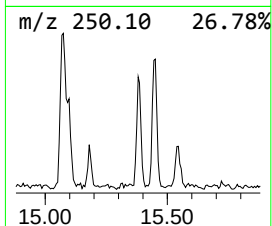
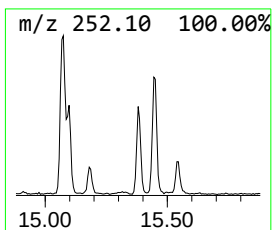
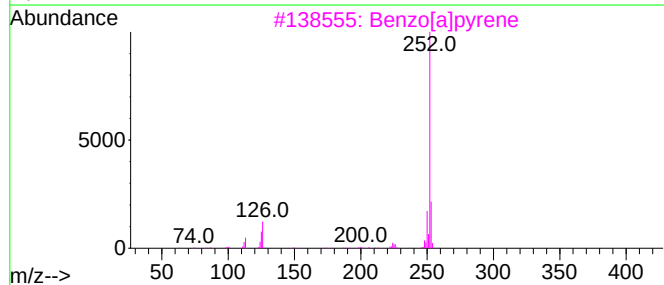
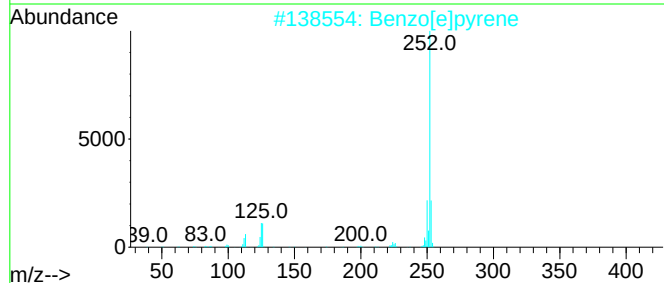
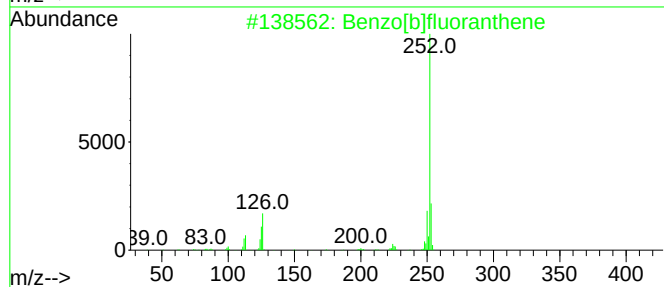
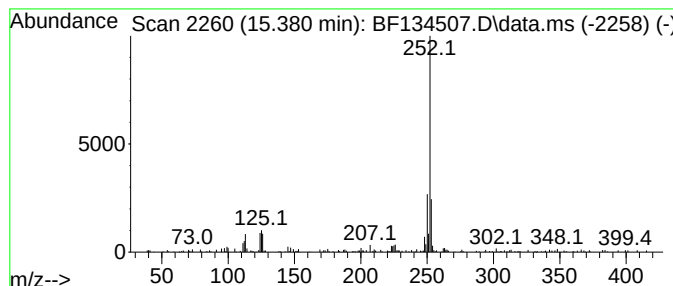
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.380	3.90 ng	62967	Perylene-d12	15.510

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]fluoranthene	252	C20H12	000205-99-2	95
2			Benzo[e]pyrene	252	C20H12	000192-97-2	90
3			Benzo[a]pyrene	252	C20H12	000050-32-8	90
4			Benzo[k]fluoranthene	252	C20H12	000207-08-9	89
5			Perylene	252	C20H12	000198-55-0	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072723\
Data File : BF134507.D
Acq On : 27 Jul 2023 15:56
Operator : CG\JU
Sample : 03736-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-5-072423

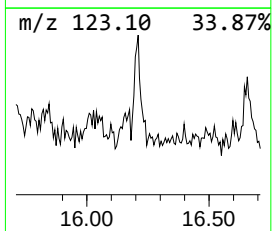
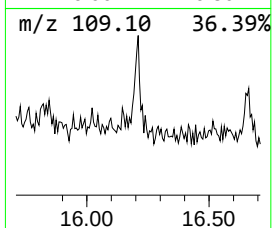
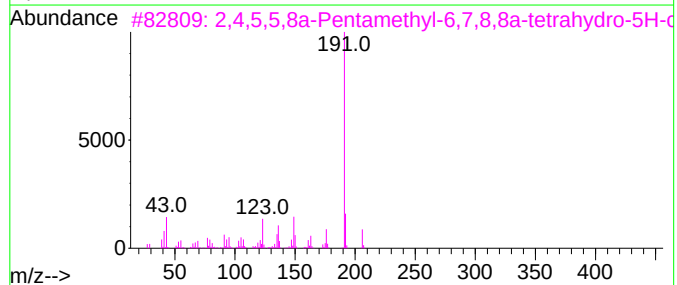
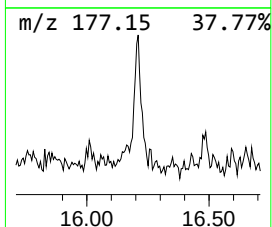
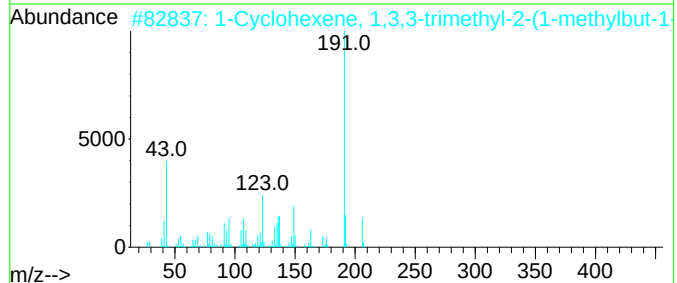
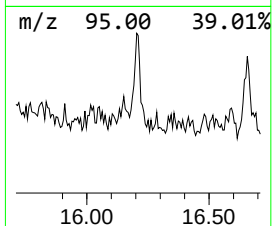
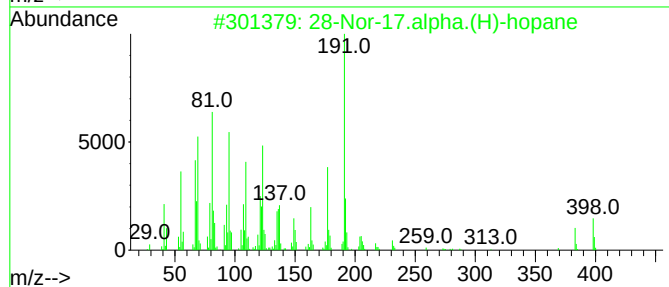
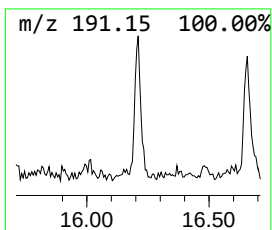
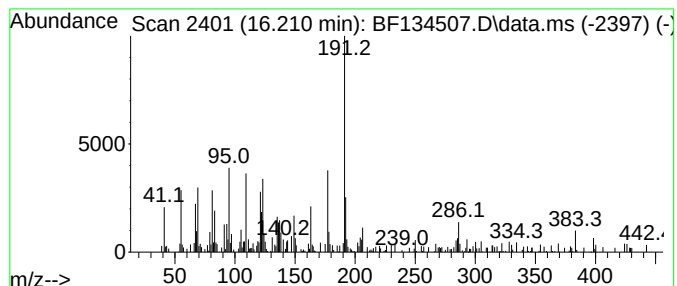
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 28-Nor-17.alpha.(H)-hopane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.210	10.28 ng	165803	Perylene-d12	15.510

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			28-Nor-17.alpha.(H)-hopane	398	C29H50	053584-60-4	93
2			1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H220	1000197-08-4	45
3			2,4,5,5,8a-Pentamethyl-6,7,8,8a...	206	C14H220	1000195-40-9	43
4			1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H220	000127-43-5	43
5			2-Fluoro-3-trifluoromethylbenzoi...	338	C10H5Cl3F402	1000357-26-6	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072723\
Data File : BF134507.D
Acq On : 27 Jul 2023 15:56
Operator : CG\JU
Sample : 03736-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	11.881	11.8	ng	292102	4	11.351	494950	20.0
4H-Cyclopenta[d]...	11.969	3.3	ng	81228	4	11.351	494950	20.0
Cyclopentane, 1...	12.433	3.7	ng	91798	4	11.351	494950	20.0
Octadecanoic acid	12.669	4.8	ng	120015	4	11.351	494950	20.0
Pyrene, 1-methyl-	13.133	2.0	ng	58641	5	14.016	583335	20.0
Stilbene, 2-hyd...	13.863	5.0	ng	145599	5	14.016	583335	20.0
Benzo[e]pyrene	15.380	3.9	ng	62967	6	15.510	322665	20.0
28-Nor-17.alpha...	16.210	10.3	ng	165803	6	15.510	322665	20.0