

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082423\
 Data File : BF134931.D
 Acq On : 24 Aug 2023 18:52
 Operator : CG\JU
 Sample : 04116-09 2X
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-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-BF082223.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134931.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.422	563	567	582	rBV	745591	742860	94.04%	7.848%
2	6.428	734	738	748	rBV	908694	766443	97.03%	8.097%
3	6.792	797	800	805	rVB	837293	672290	85.11%	7.102%
4	7.351	892	895	904	rVB	566106	442477	56.02%	4.675%
5	8.075	1014	1018	1021	rBV	971385	789918	100.00%	8.345%
6	8.134	1026	1028	1031	rVB	20049	15976	2.02%	0.169%
7	8.363	1063	1067	1070	rBV5	13759	16072	2.03%	0.170%
8	8.498	1086	1090	1092	rBV	35905	34933	4.42%	0.369%
9	8.763	1132	1135	1138	rVB4	19598	19786	2.50%	0.209%
10	9.098	1189	1192	1197	rBV2	60548	49762	6.30%	0.526%
11	9.151	1197	1201	1204	rBV	988375	767518	97.16%	8.109%
12	9.233	1211	1215	1217	rBV4	18466	22762	2.88%	0.240%
13	9.533	1264	1266	1268	rBV2	24027	21862	2.77%	0.231%
14	9.557	1268	1270	1273	rVB2	39562	28113	3.56%	0.297%
15	9.692	1290	1293	1298	rBV4	18054	21897	2.77%	0.231%
16	9.739	1298	1301	1303	rBV2	26934	19861	2.51%	0.210%
17	9.833	1313	1317	1320	rVB	851542	765091	96.86%	8.083%
18	9.933	1331	1334	1339	rBV6	14512	20658	2.62%	0.218%
19	10.033	1347	1351	1353	rVB5	20961	22583	2.86%	0.239%
20	10.151	1368	1371	1374	rBV2	16068	21231	2.69%	0.224%
21	10.333	1399	1402	1406	rVB5	20292	22346	2.83%	0.236%
22	10.380	1407	1410	1412	rBV3	16426	17372	2.20%	0.184%
23	10.492	1426	1429	1433	rVB2	36818	37795	4.78%	0.399%
24	10.539	1434	1437	1441	rVB5	16445	23905	3.03%	0.253%
25	10.622	1447	1451	1455	rBV	580165	478506	60.58%	5.055%
26	10.757	1470	1474	1477	rVB	69268	66303	8.39%	0.700%
27	10.828	1482	1486	1491	rBV7	17516	34633	4.38%	0.366%
28	11.227	1550	1554	1558	rVB2	80530	89266	11.30%	0.943%
29	11.322	1567	1570	1573	rBV	845360	775476	98.17%	8.193%
30	11.345	1573	1574	1577	rVB	38398	27405	3.47%	0.290%
31	11.857	1659	1661	1666	rVB3	95815	89095	11.28%	0.941%
32	11.939	1673	1675	1678	rBV2	38032	33271	4.21%	0.351%
33	12.257	1727	1729	1735	rBV2	62246	84221	10.66%	0.890%
34	12.386	1748	1751	1753	rBV	63197	66996	8.48%	0.708%
35	12.780	1815	1818	1825	rBV3	110052	179023	22.66%	1.891%
36	12.921	1839	1842	1845	rBV	895391	728700	92.25%	7.698%

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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-BF082223.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.369	1916	1918	1921	rBV2	123656	97968	12.40%	1.035%
38	13.986	2020	2023	2028	rVB	748655	680086	86.10%	7.185%
39	15.468	2272	2275	2286	rVB	420756	671095	84.96%	7.090%

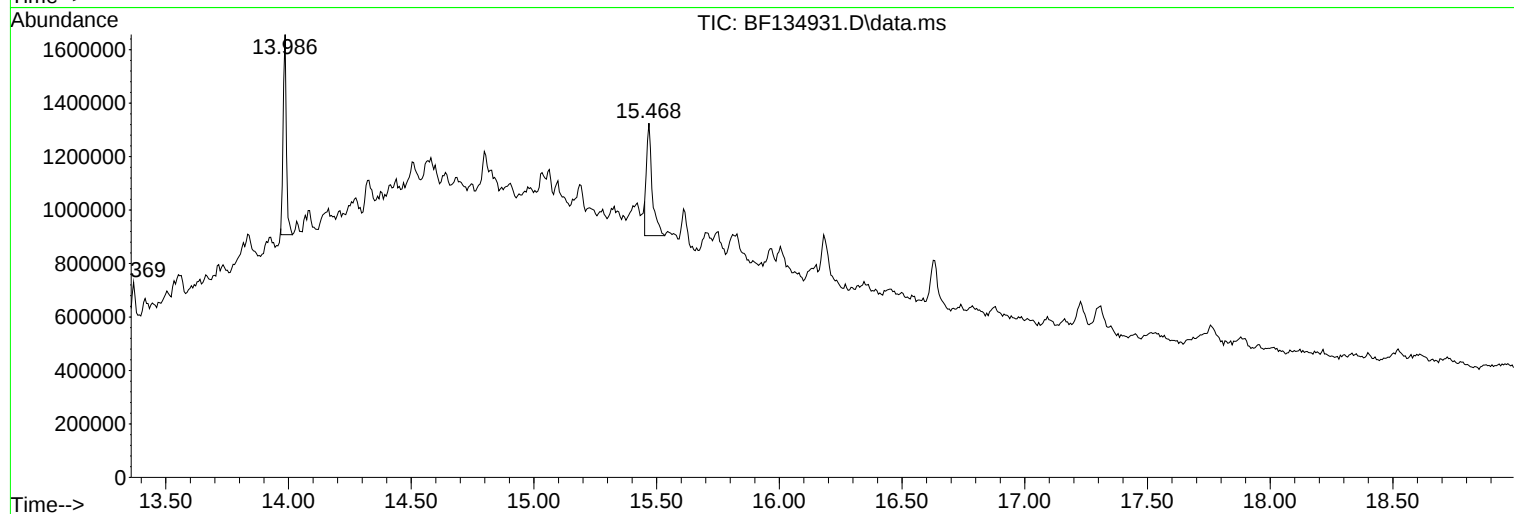
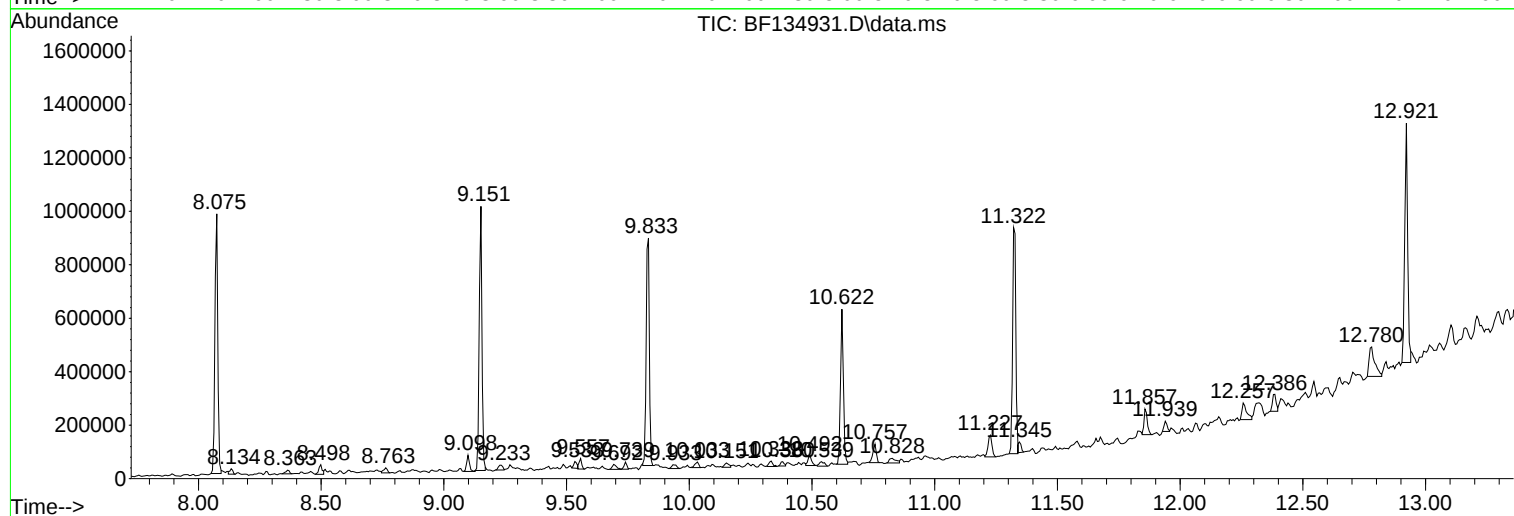
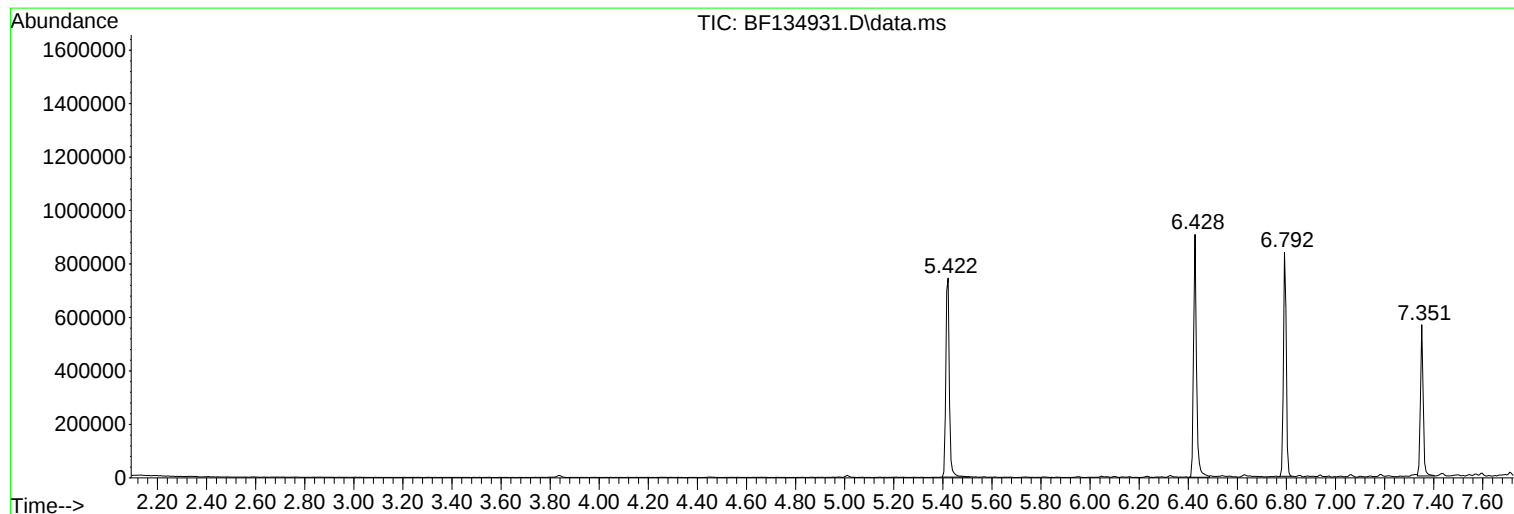
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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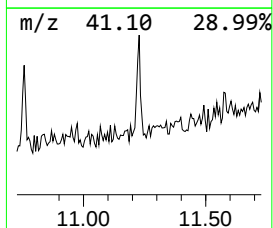
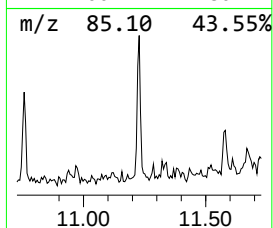
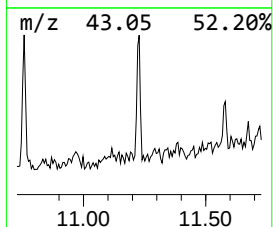
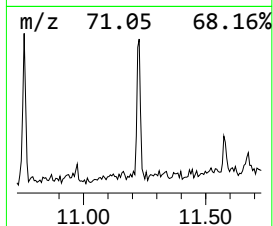
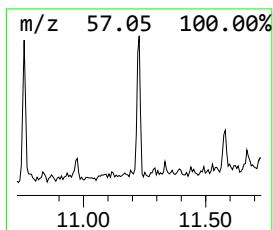
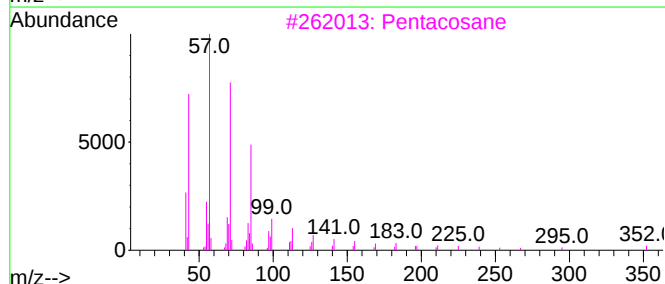
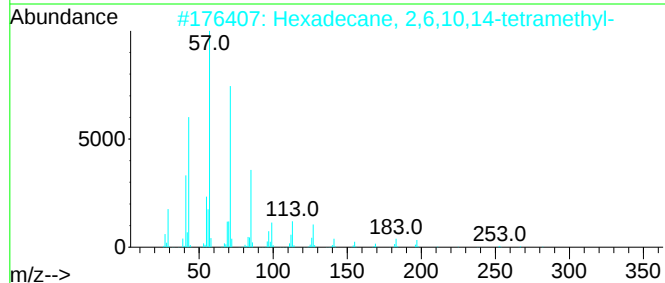
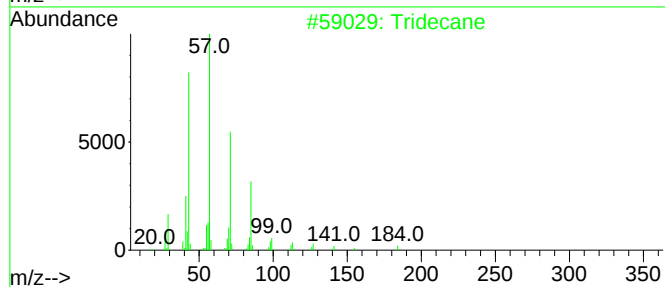
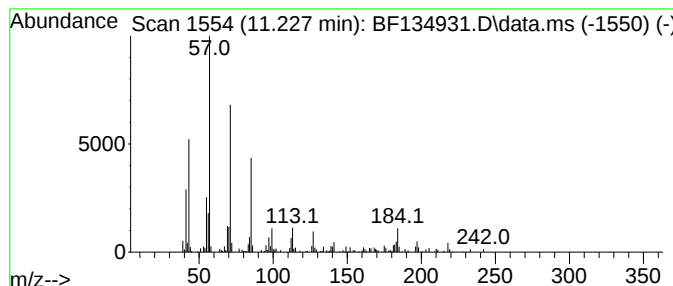
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Tridecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.227	2.30 ng	89266	Phenanthrene-d10	11.328

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	93
2			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	87
3			Pentacosane	352	C25H52	000629-99-2	83
4			Dodecane, 3-methyl-	184	C13H28	017312-57-1	83
5			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	81



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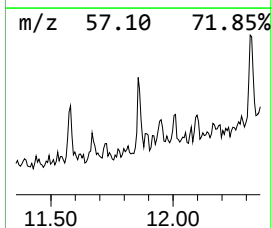
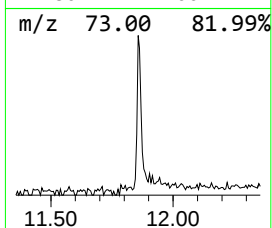
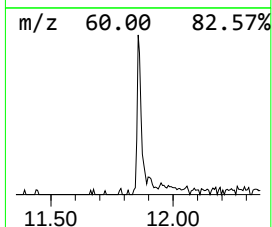
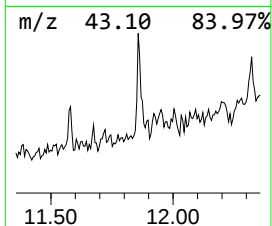
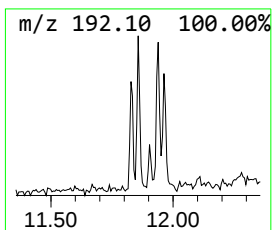
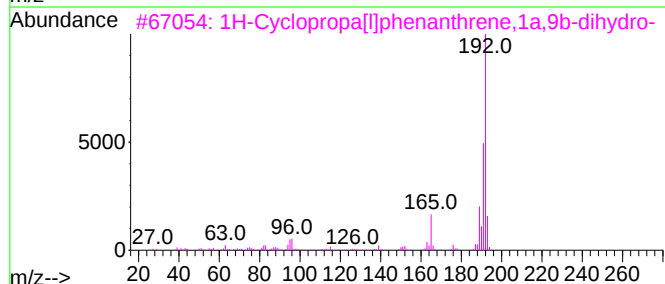
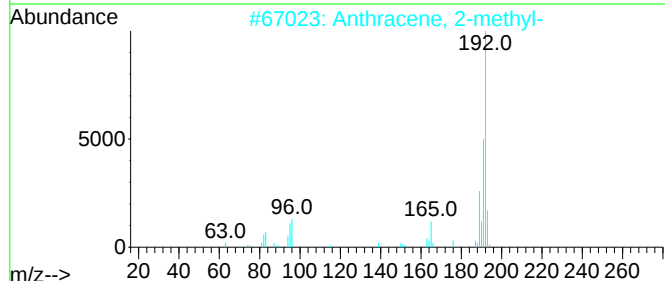
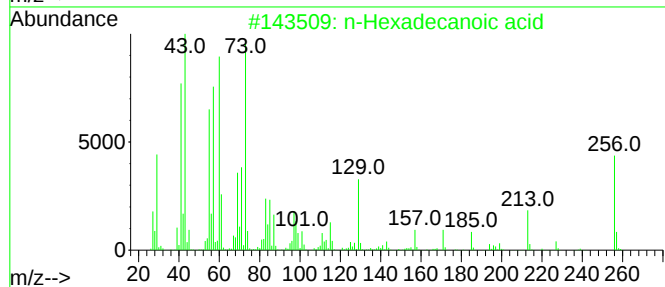
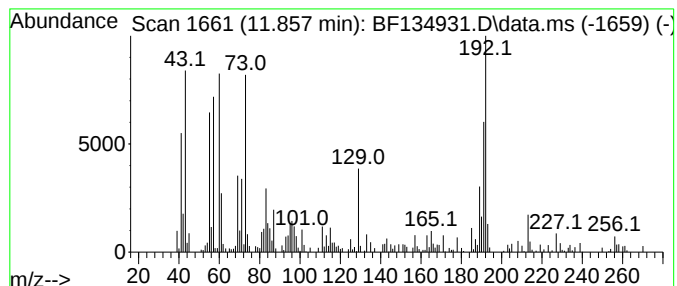
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	2.30 ng	89095	Phenanthrene-d10	11.328

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	55
2			Anthracene, 2-methyl-	192	C15H12	000613-12-7	45
3			1H-Cyclopropa[1]phenanthrene,1a,...	192	C15H12	000949-41-7	38
4			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	38
5			Anthracene, 9-methyl-	192	C15H12	000779-02-2	38



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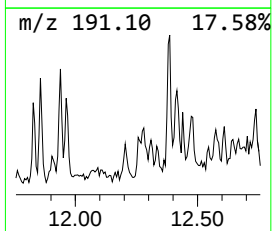
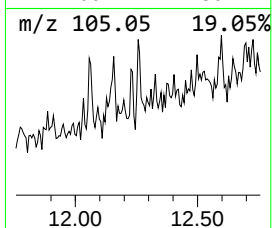
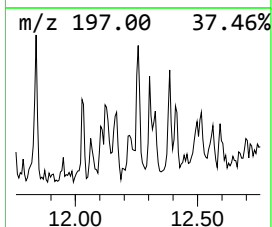
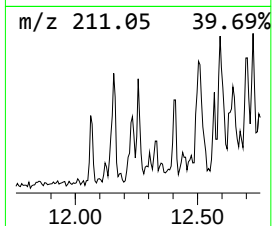
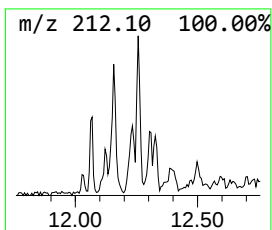
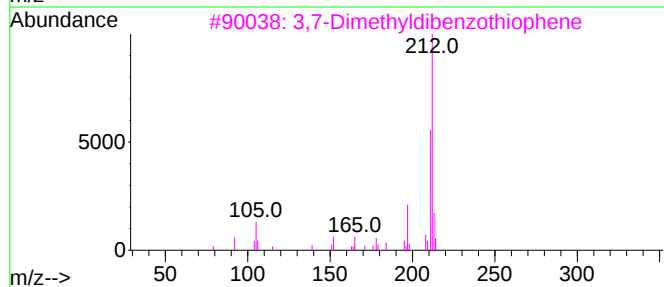
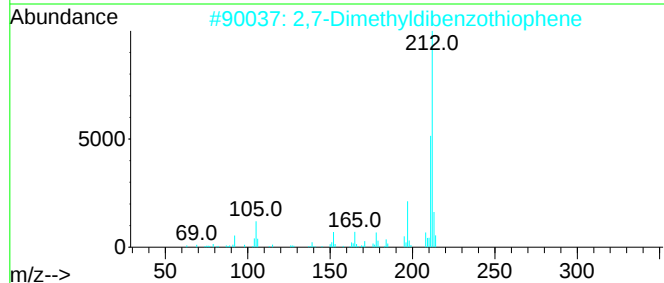
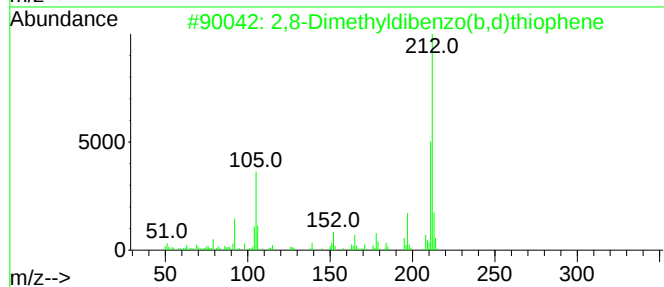
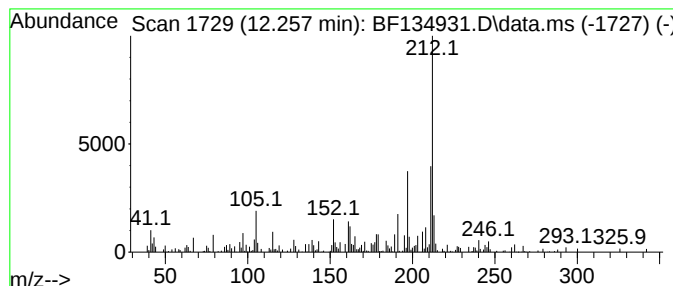
Instrument :
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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2,8-Dimethyldibenzo(b,d)thi... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.257	2.17 ng	84221	Phenanthrene-d10		11.328	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2,8-Dimethyldibenzo(b,d)thiophene		212	C14H12S	001207-15-4	80
2	2,7-Dimethyldibenzothiophene		212	C14H12S	031317-19-8	76
3	3,7-Dimethyldibenzothiophene		212	C14H12S	001136-85-2	76
4	2,6-Dimethyldibenzothiophene		212	C14H12S	089816-75-1	76
5	Naphtho[2,3-b]thiophene, 4,9-dim...		212	C14H12S	016587-34-1	72



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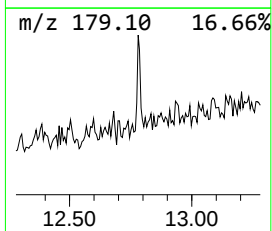
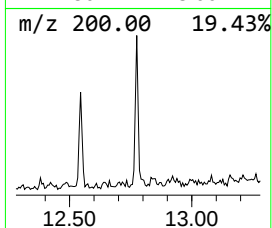
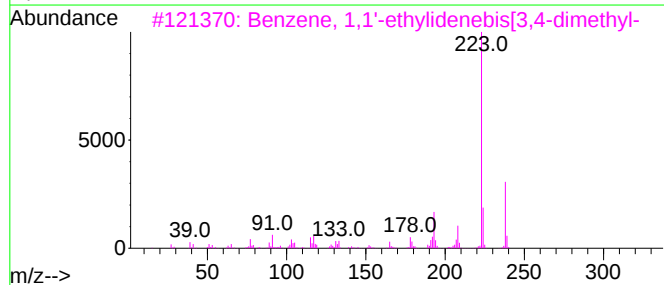
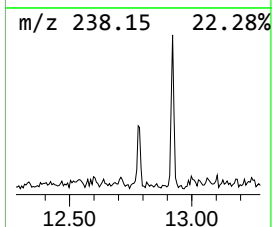
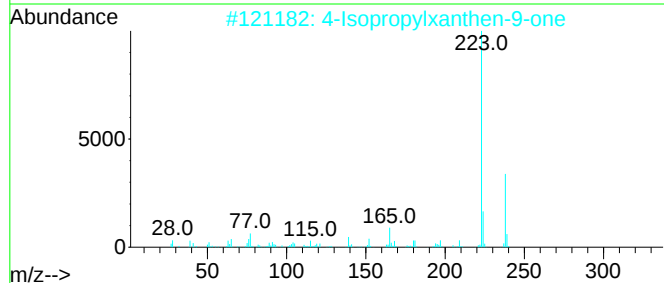
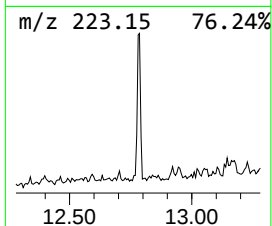
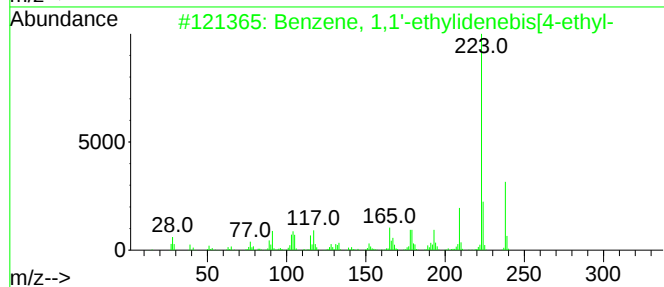
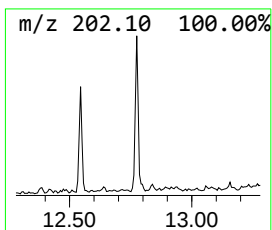
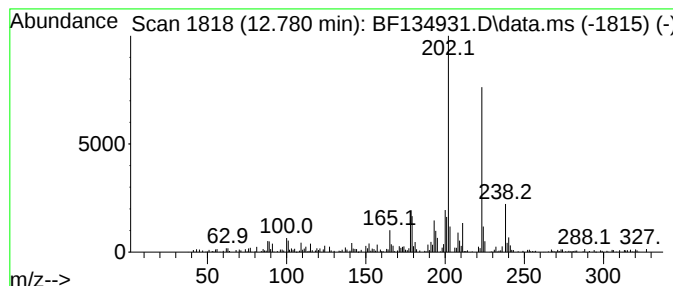
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown12.780 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.780	5.26 ng	179023	Chrysene-d12	13.986

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,1'-ethylidenebis[4-et...	238	C18H22	010224-91-6	46
2			4-Isopropylxanthen-9-one	238	C16H14O2	1000210-33-1	46
3			Benzene, 1,1'-ethylidenebis[3,4-...	238	C18H22	001742-14-9	46
4			Indeno[2,1-c]pyridin-9-one, 3,5,...	223	C15H13NO	064322-97-0	42
5			1,4,7-Trimethyl-2-azafluorenone	223	C15H13NO	064322-98-1	42



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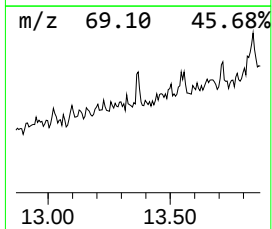
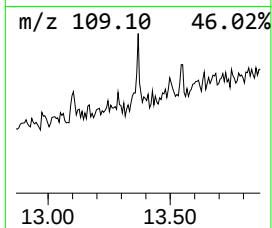
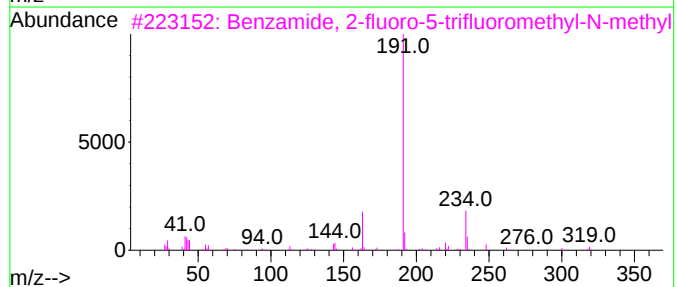
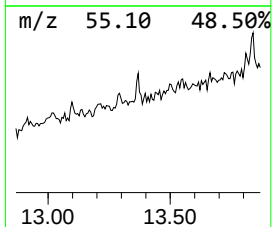
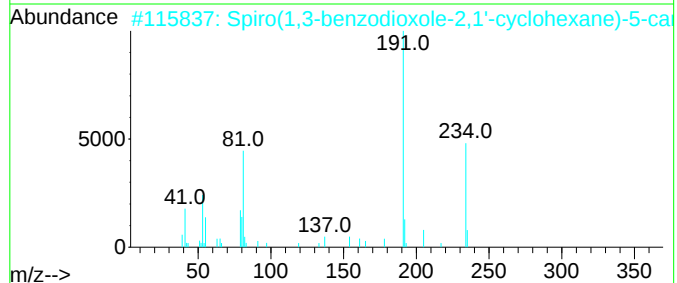
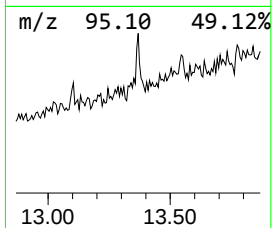
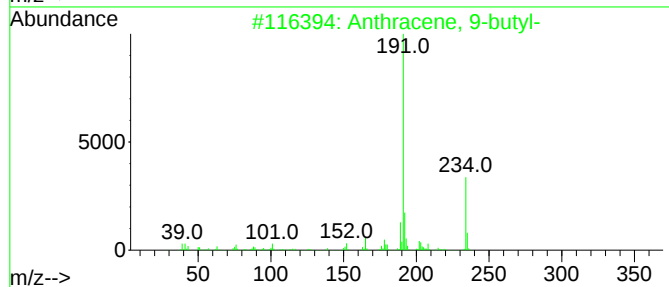
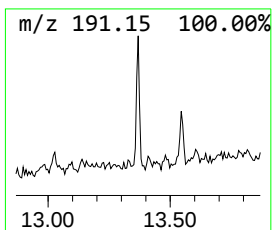
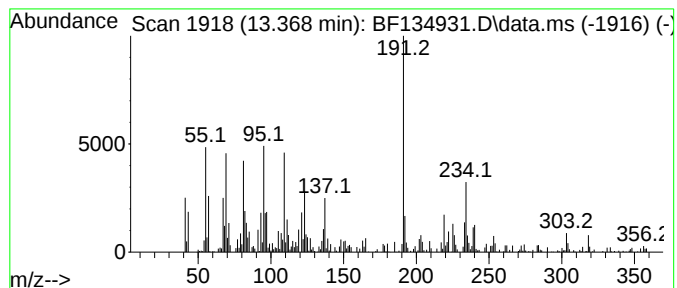
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown13.368 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.368	2.88 ng	97968	Chrysene-d12	13.986

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Anthracene, 9-butyl-	234	C18H18	001498-69-7	38
2			Spiro(1,3-benzodioxole-2,1'-cycl...	234	C13H14O4	056011-74-6	38
3			Benzamide, 2-fluoro-5-trifluorom...	319	C16H21F4NO	1000437-13-2	30
4			Benzamide, 2-fluoro-3-trifluorom...	319	C16H21F4NO	1000437-10-0	30
5			Benzamide, 2-fluoro-3-trifluorom...	347	C18H25F4NO	1000437-10-2	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082423\
Data File : BF134931.D
Acq On : 24 Aug 2023 18:52
Operator : CG\JU
Sample : 04116-09 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082223.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
Tridecane	11.227	2.3	ng	89266	4	11.328	775476	20.0
n-Hexadecanoic ...	11.857	2.3	ng	89095	4	11.328	775476	20.0
2,8-Dimethyldib...	12.257	2.2	ng	84221	4	11.328	775476	20.0
unknown12.780	12.780	5.3	ng	179023	5	13.986	680086	20.0
unknown13.368	13.368	2.9	ng	97968	5	13.986	680086	20.0