

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012622\
 Data File : BF126703.D
 Acq On : 26 Jan 2022 22:45
 Operator : CG/JU
 Sample : N1266-08
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RB-11-(2.10-3.6)

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-BF011822.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126703.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.304	29	37	44	rVB	469582	615058	14.66%	1.927%
2	5.192	523	528	534	rVB	143546	170196	4.06%	0.533%
3	5.575	588	593	596	rBV	4187045	3967148	94.54%	12.429%
4	6.569	756	762	765	rBV	3971061	4196112	100.00%	13.147%
5	6.951	824	827	831	rVB	1155787	1042869	24.85%	3.267%
6	7.516	918	923	926	rBV	2879773	2669080	63.61%	8.362%
7	8.128	1024	1027	1038	rBV	63855	74336	1.77%	0.233%
8	8.233	1041	1045	1049	rBV	1425532	1392965	33.20%	4.364%
9	9.316	1223	1229	1232	rBV	4411707	4111883	97.99%	12.883%
10	9.386	1236	1241	1243	rBV	58503	50611	1.21%	0.159%
11	9.857	1318	1321	1325	rVB	82459	63400	1.51%	0.199%
12	9.998	1341	1345	1348	rBV	1787546	1549603	36.93%	4.855%
13	10.786	1475	1479	1482	rBV	2678284	2285158	54.46%	7.160%
14	11.486	1594	1598	1601	rBV	1739591	1538773	36.67%	4.821%
15	11.510	1601	1602	1606	rVB	130318	86464	2.06%	0.271%
16	12.098	1699	1702	1705	rBV2	40882	46366	1.10%	0.145%
17	12.704	1802	1805	1809	rVB	297316	240929	5.74%	0.755%
18	12.933	1839	1844	1848	rBV	332499	312703	7.45%	0.980%
19	13.080	1864	1869	1872	rBV	3823168	3382143	80.60%	10.597%
20	13.151	1878	1881	1885	rBV4	35764	51286	1.22%	0.161%
21	13.368	1915	1918	1921	rVB	56994	46563	1.11%	0.146%
22	13.768	1983	1986	1990	rVB	38286	42482	1.01%	0.133%
23	13.886	1999	2006	2008	rBV2	33393	51329	1.22%	0.161%
24	13.980	2018	2022	2032	rVB5	96690	212476	5.06%	0.666%
25	14.133	2040	2048	2051	rBV2	1032124	1140076	27.17%	3.572%
26	14.162	2051	2053	2058	rVB	179575	168436	4.01%	0.528%
27	14.521	2110	2114	2118	rVB2	55526	58353	1.39%	0.183%
28	14.904	2175	2179	2187	rBV	132854	177895	4.24%	0.557%
29	15.004	2192	2196	2200	rBV3	63327	79386	1.89%	0.249%
30	15.204	2225	2230	2233	rBV2	154493	246867	5.88%	0.773%
31	15.315	2246	2249	2254	rBV	46986	55769	1.33%	0.175%
32	15.521	2280	2284	2290	rVB	122785	151328	3.61%	0.474%
33	15.586	2290	2295	2301	rVB2	182156	245706	5.86%	0.770%
34	15.656	2302	2307	2311	rBV	723017	941138	22.43%	2.949%
35	15.886	2342	2346	2354	rVB7	20522	46202	1.10%	0.145%
36	17.033	2534	2541	2549	rVB7	19613	50713	1.21%	0.159%

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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-BF011822.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	17.203	2563	2570	2580	rVB3	76004	164137	3.91%	0.514%
38	17.462	2610	2614	2629	rVB6	20763	53800	1.28%	0.169%
39	17.674	2643	2650	2657	rBV3	63897	137628	3.28%	0.431%

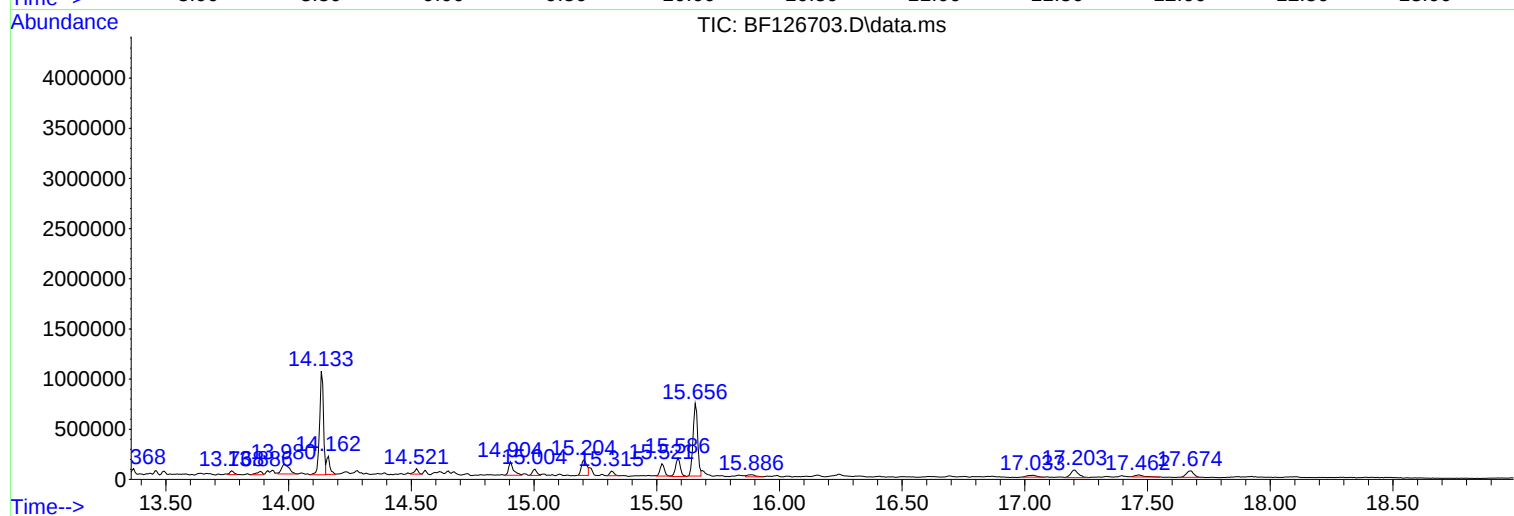
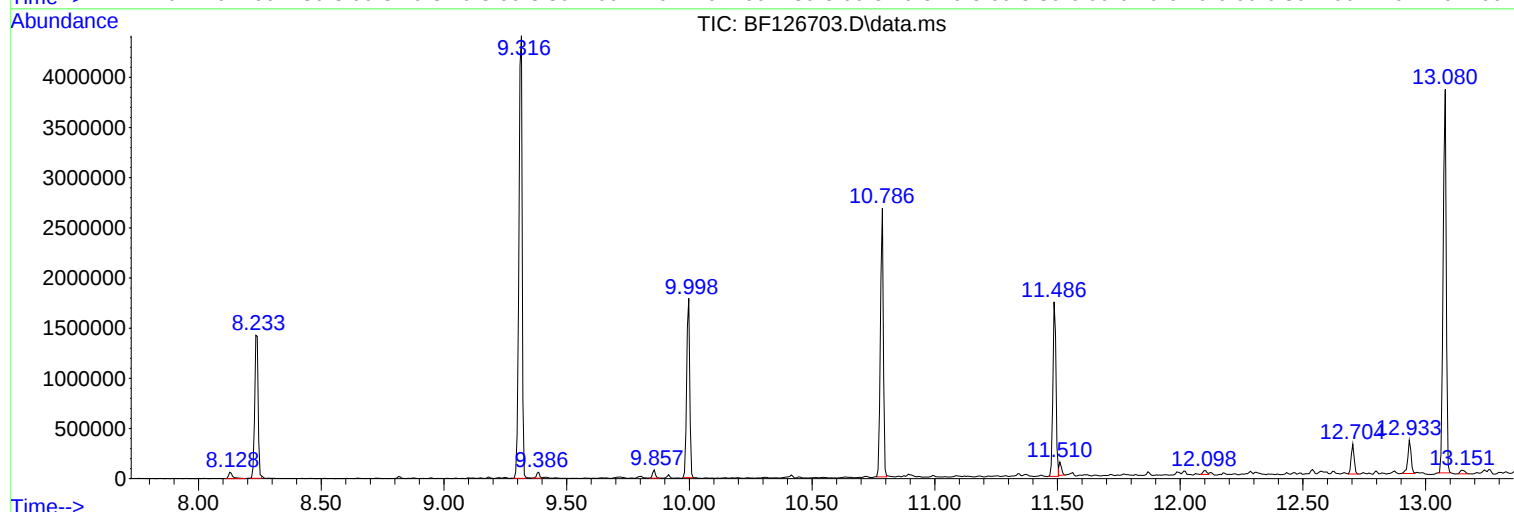
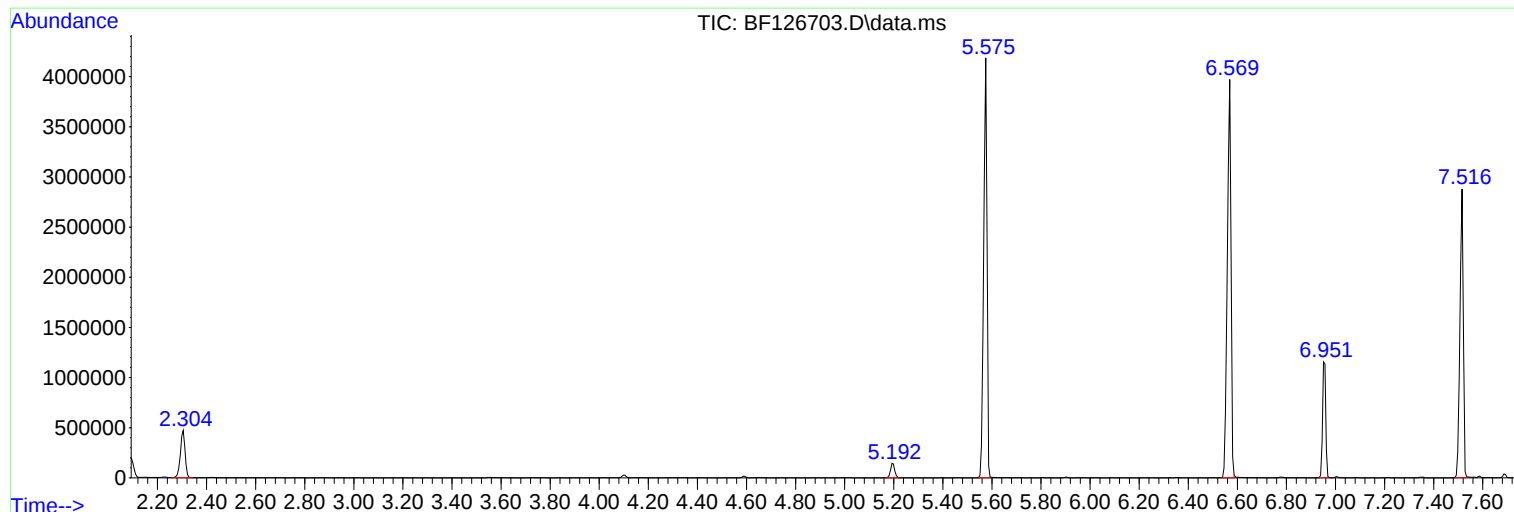
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Instrument :
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RB-11-(2.10-3.6)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.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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Misc :
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Instrument :
BNA_F
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RB-11-(2.10-3.6)

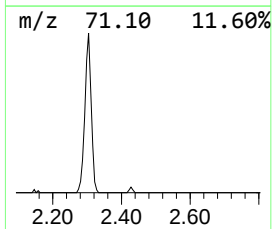
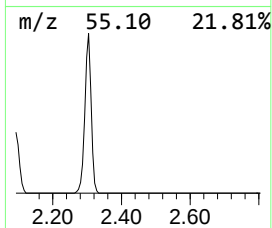
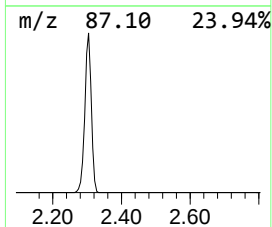
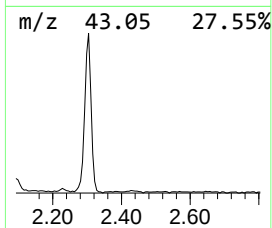
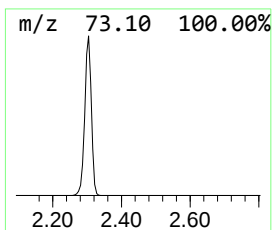
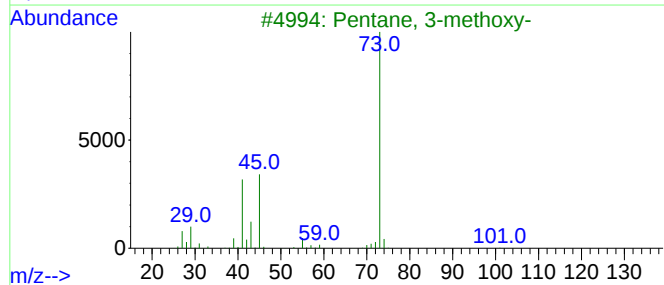
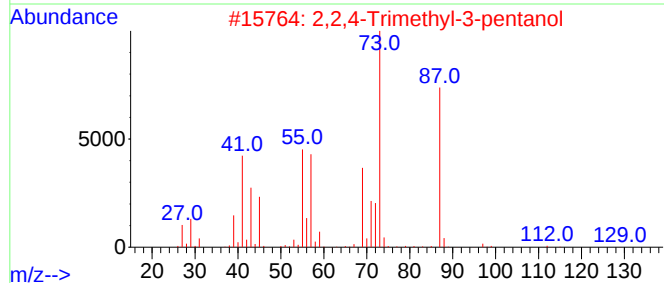
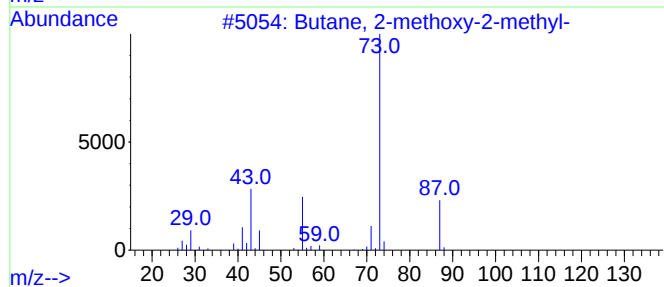
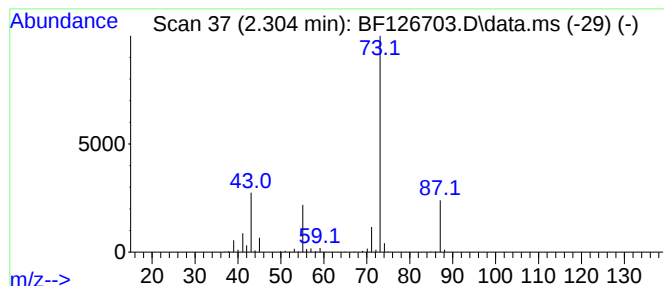
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.304	11.80 ng	615058	1,4-Dichlorobenzene-d4	6.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	16
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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Sample : N1266-08
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-11-(2.10-3.6)

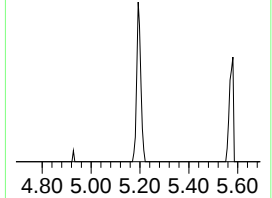
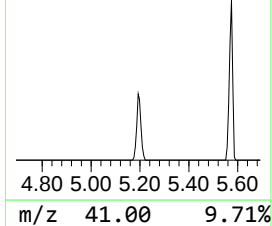
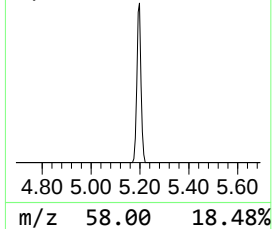
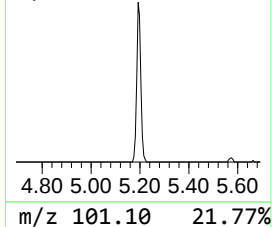
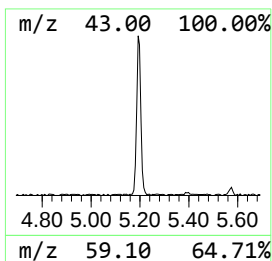
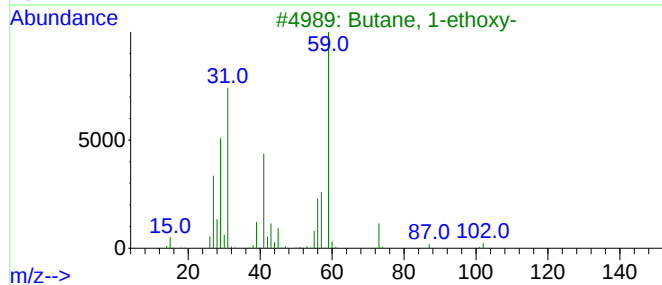
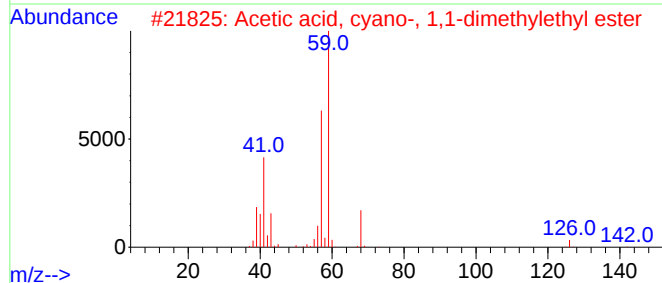
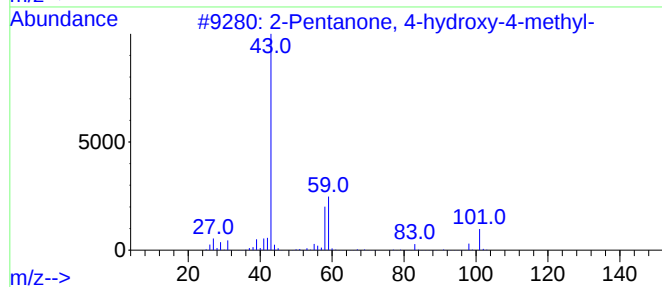
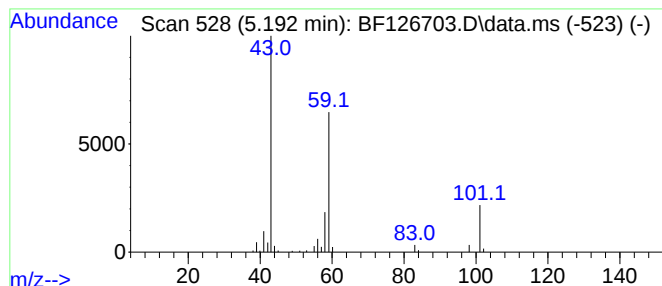
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.192	3.26 ng	170196	1,4-Dichlorobenzene-d4	6.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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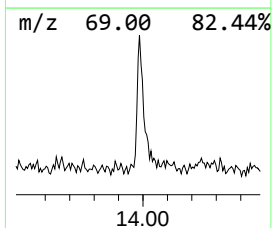
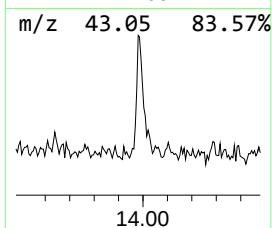
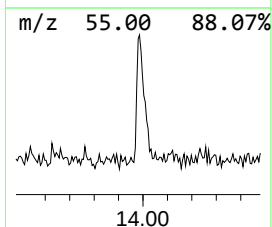
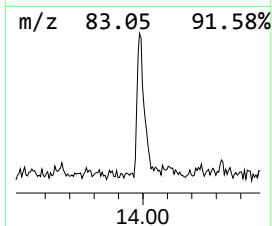
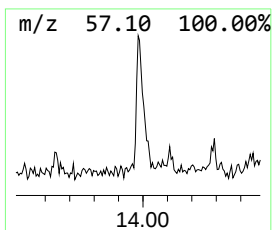
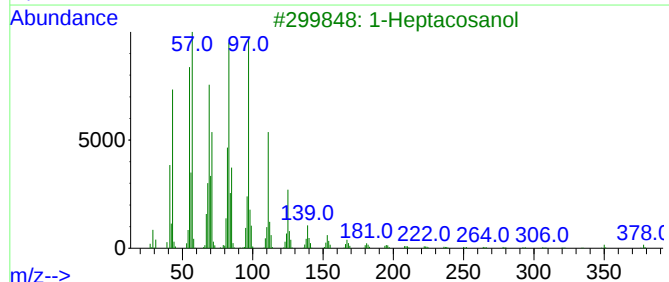
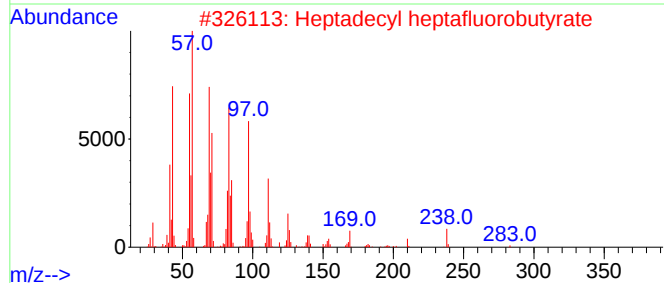
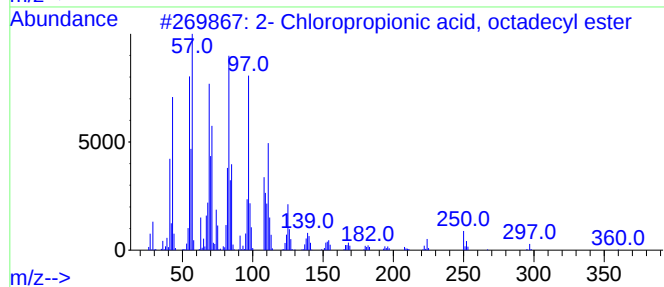
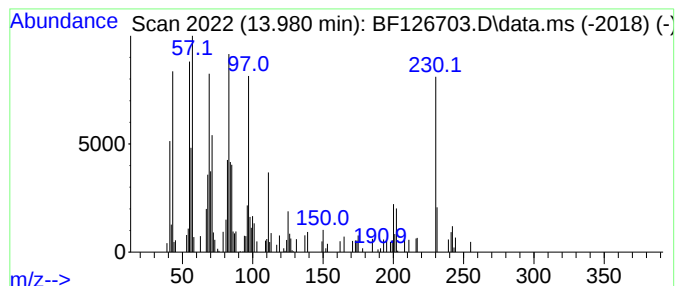
Instrument :
BNA_F
ClientSampleId :
RB-11-(2.10-3.6)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2- Chloropropionic acid, oc... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.980	3.73 ng	212476	Chrysene-d12	14.133	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	64
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	64
3	1-Heptacosanol	396	C27H56O	002004-39-9	64
4	Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	64
5	1-Tricosene	322	C23H46	018835-32-0	60



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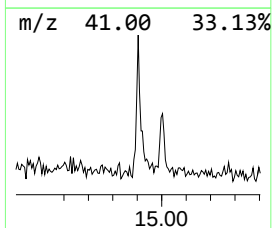
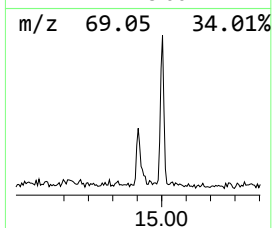
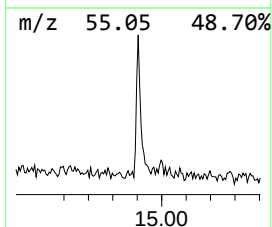
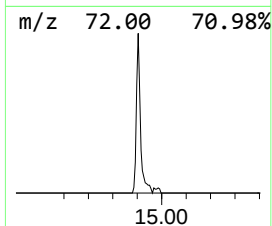
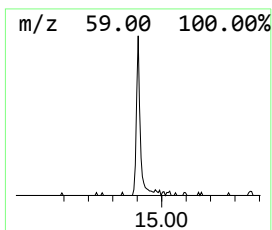
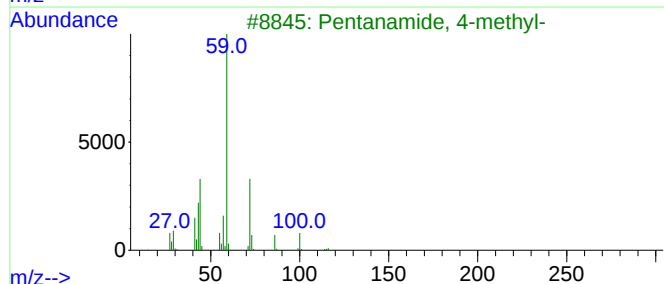
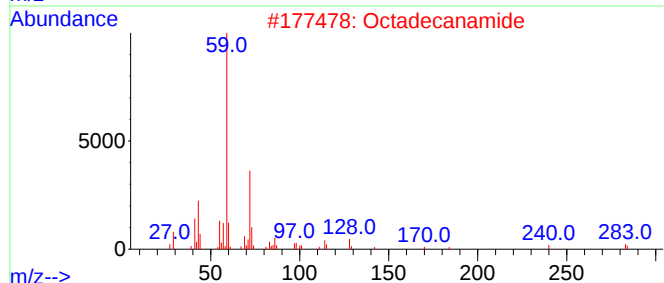
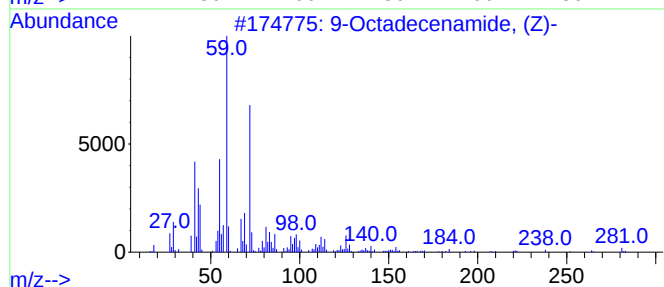
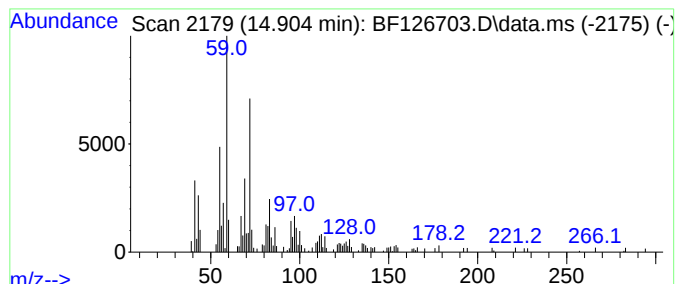
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.904	3.78 ng	177895	Perylene-d12	15.656

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	80
2			Octadecanamide	283	C18H37NO	000124-26-5	60
3			Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	53
4			Decanamide-	171	C10H21NO	002319-29-1	50
5			7-Nonenamide	155	C9H17NO	090949-53-4	46



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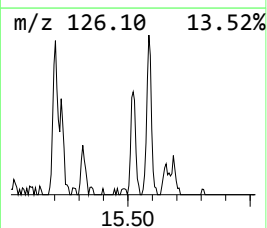
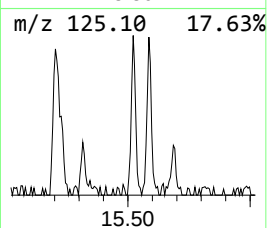
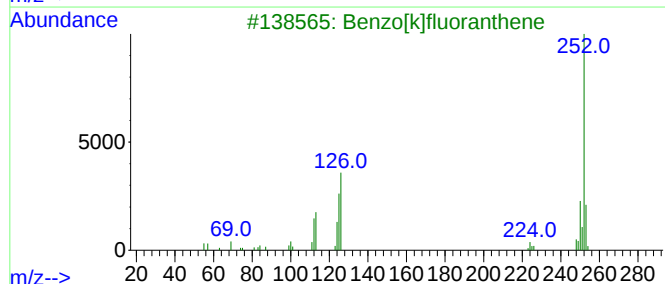
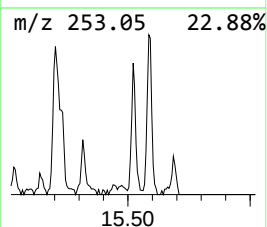
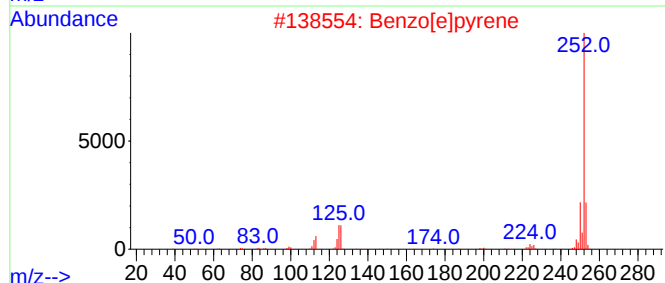
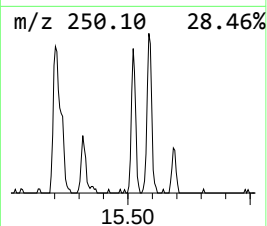
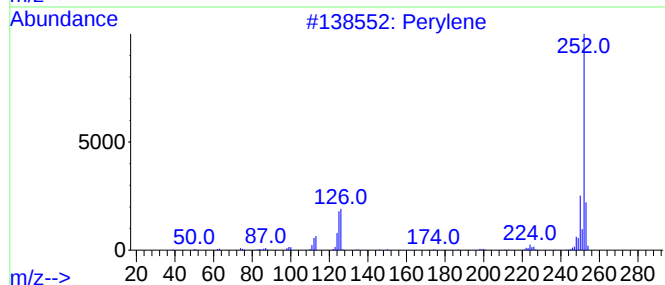
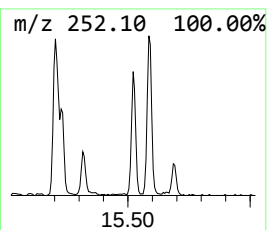
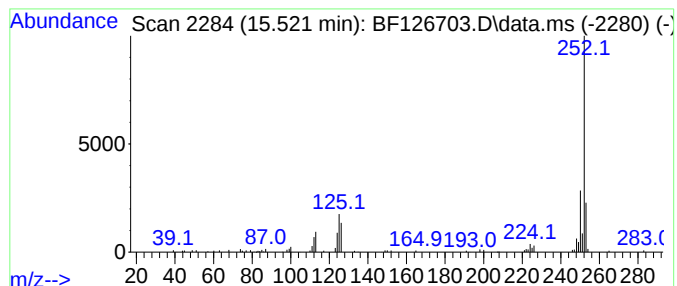
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Perylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.521	3.22 ng	151328	Perylene-d12	15.656

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	97
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
4			Benzo[j]fluoranthene	252	C20H12	000205-82-3	94
5			Benzo[b]fluoranthene	252	C20H12	000205-99-2	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012622\
Data File : BF126703.D
Acq On : 26 Jan 2022 22:45
Operator : CG/JU
Sample : N1266-08
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-11-(2.10-3.6)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.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
Butane, 2-metho...	2.304	11.8	ng	615058	1	6.957	1042870	20.0
2-Pentanone, 4-...	5.192	3.3	ng	170196	1	6.957	1042870	20.0
2-Chloropropio...	13.980	3.7	ng	212476	5	14.133	1140080	20.0
9-Octadecenamid...	14.904	3.8	ng	177895	6	15.656	941138	20.0
Perylene	15.521	3.2	ng	151328	6	15.656	941138	20.0