

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071222\
 Data File : BF129189.D
 Acq On : 12 Jul 2022 15:05
 Operator : CG\JU
 Sample : N3662-05
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20220498B-SIM/C4B-COMPOSITE

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-BF062922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129189.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.328	3	7	20	rVB	3215784	4316499	59.16%	7.846%
2	3.634	226	229	241	rBV4	27737	90742	1.24%	0.165%
3	5.198	492	495	504	rVB	77707	97240	1.33%	0.177%
4	5.569	552	558	561	rBV	6718420	6979261	95.66%	12.686%
5	6.563	720	727	730	rBV	6010558	7253807	99.42%	13.185%
6	6.669	741	745	750	rBV	81728	83637	1.15%	0.152%
7	6.934	786	790	793	rVB	2160122	1771703	24.28%	3.220%
8	7.498	880	886	889	rVB	4410451	4528938	62.07%	8.232%
9	7.563	893	897	902	rVB4	56048	84229	1.15%	0.153%
10	8.216	1001	1008	1011	rBV	2698051	2418747	33.15%	4.396%
11	8.416	1035	1042	1048	rBV7	42591	74615	1.02%	0.136%
12	8.628	1075	1078	1080	rBV	112221	98882	1.36%	0.180%
13	9.228	1177	1180	1185	rVB	169594	158143	2.17%	0.287%
14	9.292	1185	1191	1194	rBV	7635008	7295992	100.00%	13.261%
15	9.369	1200	1204	1206	rBV2	83833	93499	1.28%	0.170%
16	9.680	1253	1257	1260	rBV	283490	252747	3.46%	0.459%
17	9.833	1280	1283	1286	rBV2	87832	80652	1.11%	0.147%
18	9.880	1286	1291	1294	rVV2	76699	97208	1.33%	0.177%
19	9.975	1301	1307	1310	rVB	2928259	2463730	33.77%	4.478%
20	10.380	1372	1376	1380	rBV4	72176	91563	1.25%	0.166%
21	10.610	1412	1415	1418	rBV	186063	170728	2.34%	0.310%
22	10.769	1434	1442	1445	rBV	4353925	4366385	59.85%	7.936%
23	10.880	1456	1461	1464	rBV	331112	356110	4.88%	0.647%
24	11.345	1536	1540	1546	rVB	222831	247244	3.39%	0.449%
25	11.463	1556	1560	1563	rBV	2372778	2193375	30.06%	3.987%
26	11.486	1563	1564	1568	rVV	111029	89024	1.22%	0.162%
27	11.527	1568	1571	1576	rVB2	111788	148313	2.03%	0.270%
28	11.692	1597	1599	1603	rBV2	85530	82768	1.13%	0.150%
29	11.845	1622	1625	1628	rVB	151568	122361	1.68%	0.222%
30	11.980	1644	1648	1653	rBV2	150312	191674	2.63%	0.348%
31	12.680	1764	1767	1770	rBV	148275	119518	1.64%	0.217%
32	12.716	1771	1773	1777	rVB2	99551	88016	1.21%	0.160%
33	12.910	1804	1806	1813	rVB	156699	160060	2.19%	0.291%
34	13.051	1826	1830	1834	rVB	5217319	5153440	70.63%	9.367%
35	13.304	1871	1873	1876	rVB	84438	75651	1.04%	0.138%
36	13.986	1983	1989	1998	rBV7	71522	257391	3.53%	0.468%

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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-BF062922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.110	2006	2010	2013	rBV	1032223	1013142	13.89%	1.841%
38	14.139	2013	2015	2018	rVB	160754	121838	1.67%	0.221%
39	14.204	2020	2026	2030	rBV	655876	738228	10.12%	1.342%
40	15.627	2263	2268	2277	rVB	782947	990360	13.57%	1.800%

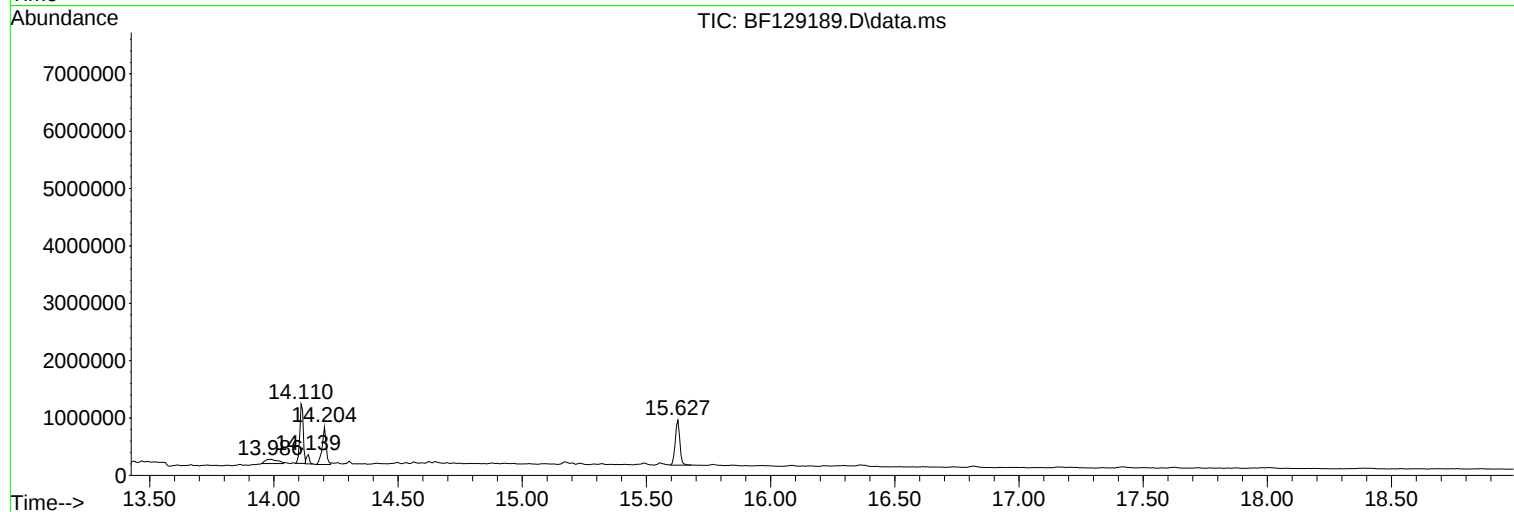
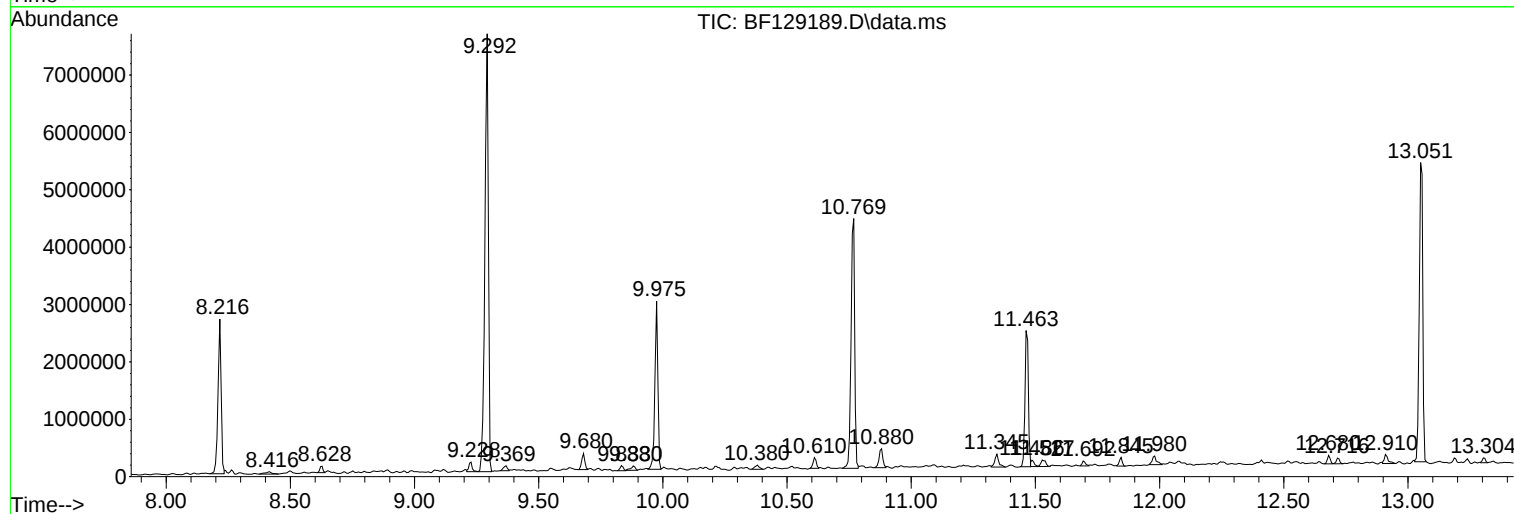
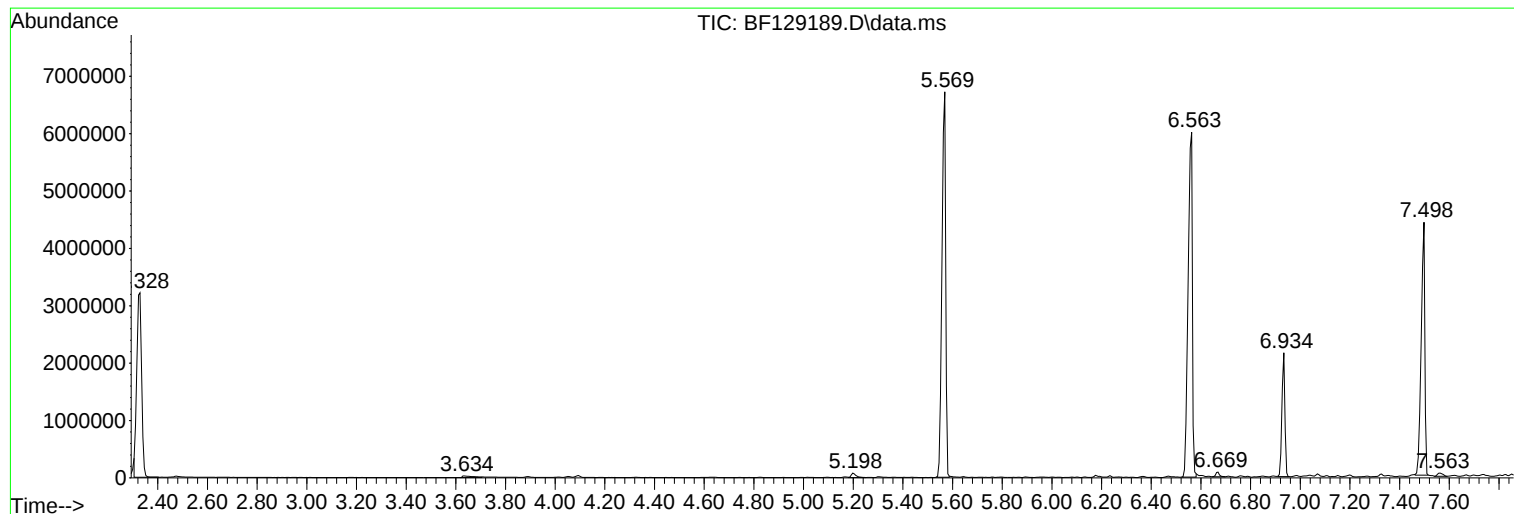
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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20220498B-SIM/C4B-COMPOSITE

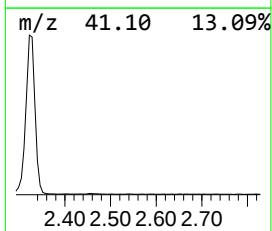
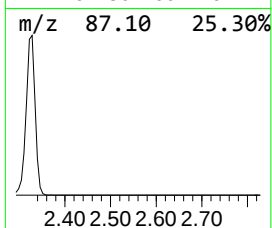
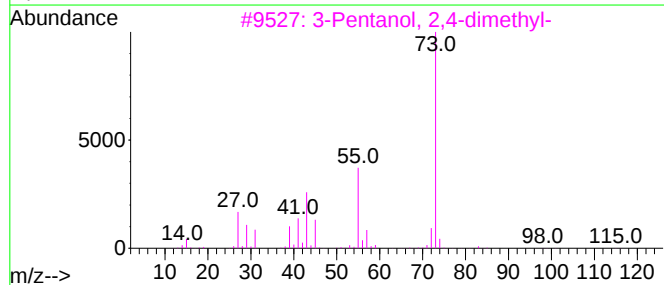
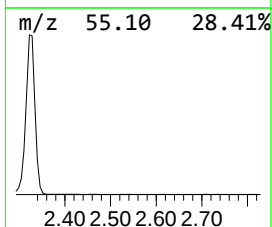
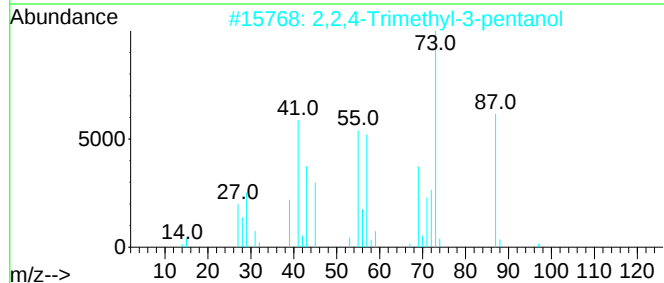
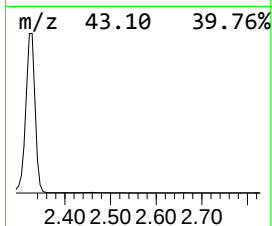
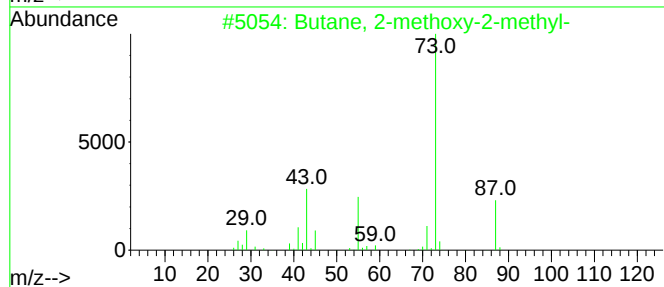
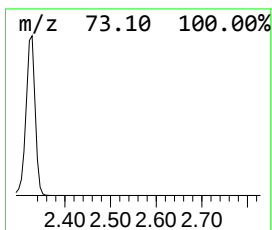
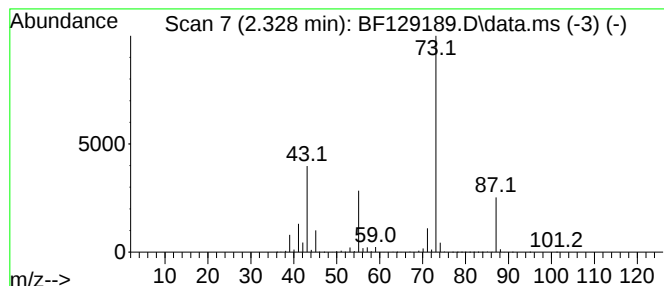
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.328	48.73 ng	4316500	1,4-Dichlorobenzene-d4	6.934

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	39
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25



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BNA_F
ClientSampleId :
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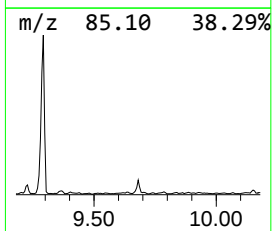
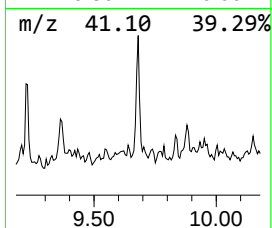
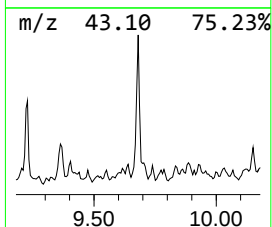
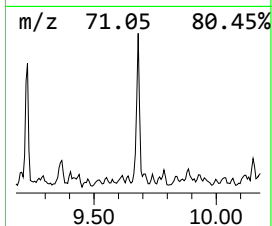
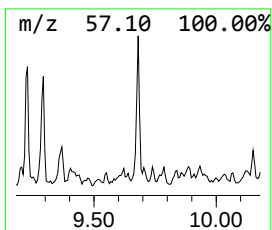
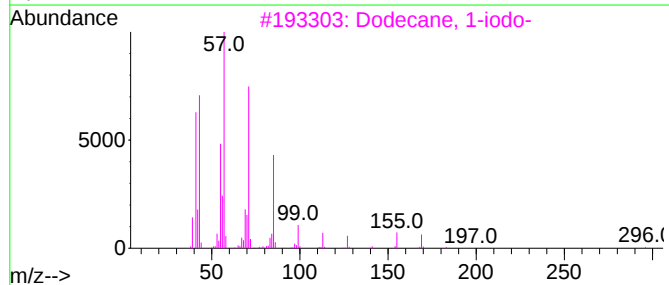
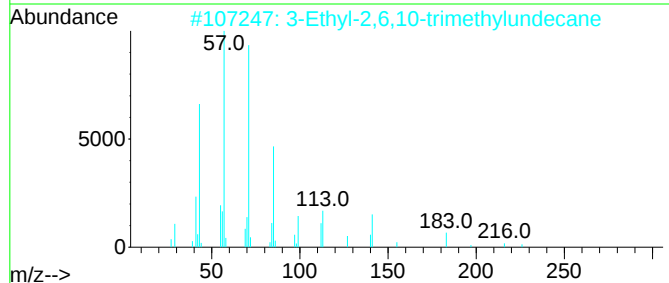
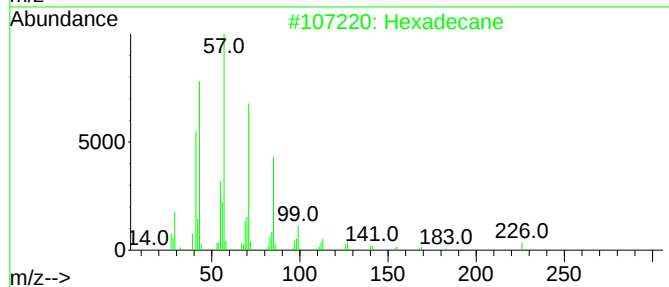
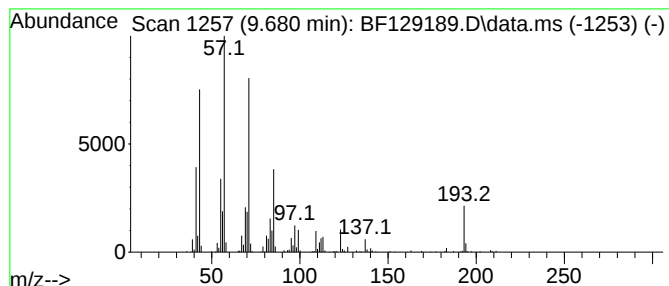
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.680	2.05 ng	252747	Acenaphthene-d10	9.975

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	64
2			3-Ethyl-2,6,10-trimethylundecane	226	C16H34	1000432-25-9	59
3			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	59
4			Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	58
5			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	58



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ALS Vial : 8 Sample Multiplier: 1

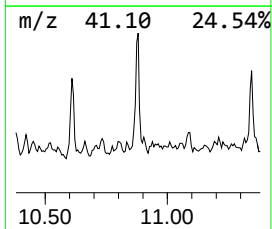
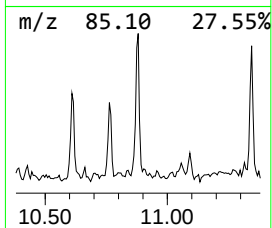
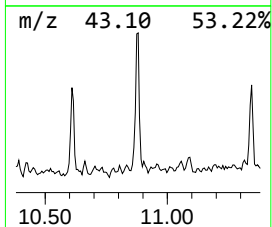
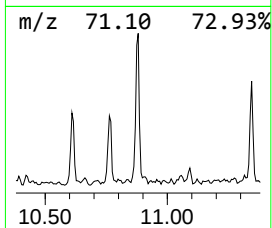
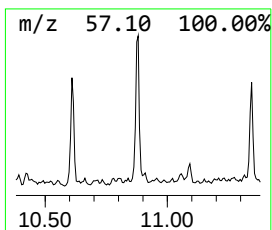
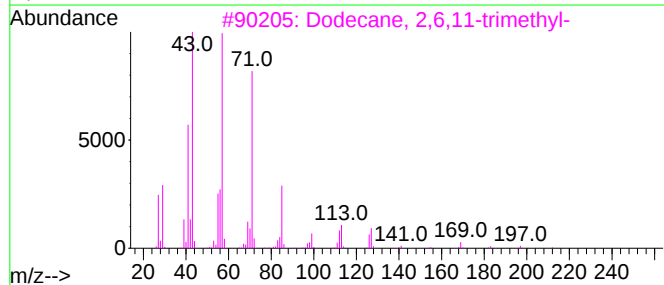
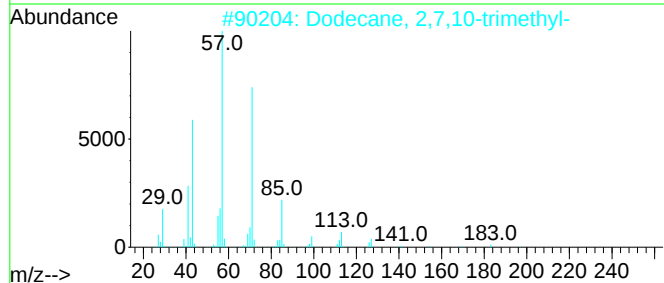
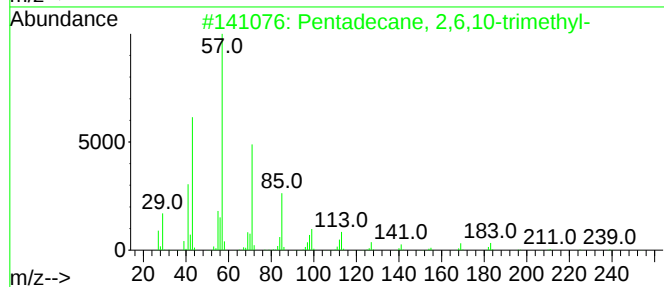
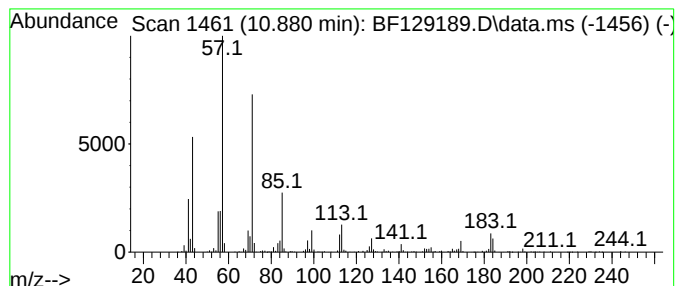
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Pentadecane, 2,6,10-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.880	3.25 ng	356110	Phenanthrene-d10	11.463	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	86
2	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	72
3	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	72
4	Undecane, 2-methyl-	170	C12H26	007045-71-8	68
5	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	68



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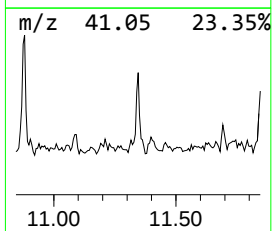
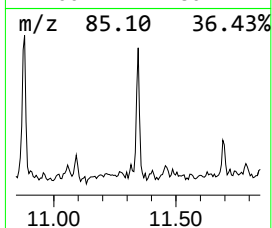
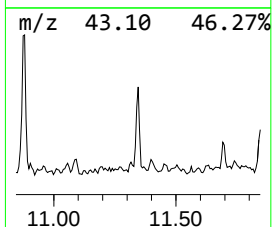
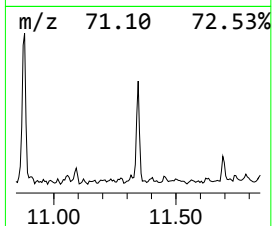
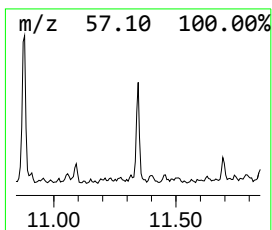
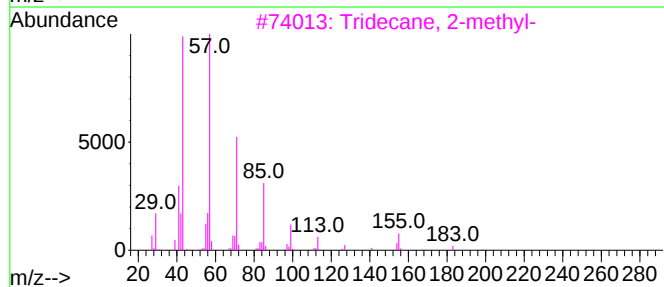
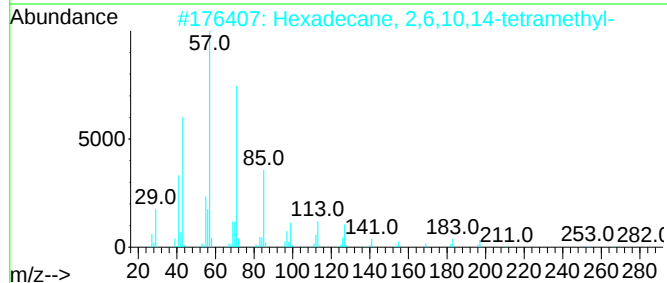
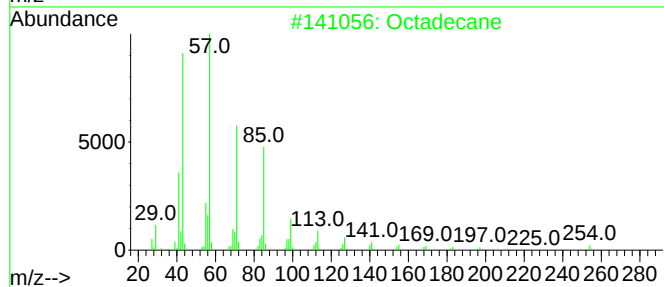
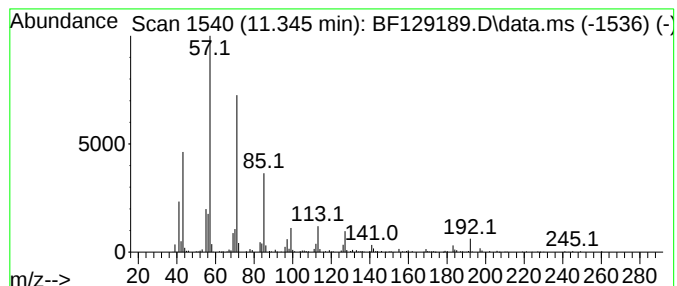
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.345	2.25 ng	247244	Phenanthrene-d10	11.463

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecane	254	C18H38	000593-45-3	86
2		Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	86
3		Tridecane, 2-methyl-	198	C14H30	001560-96-9	74
4		Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	72
5		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	72



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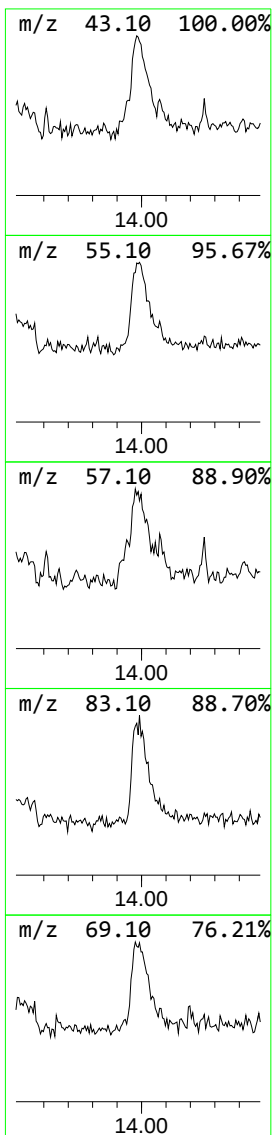
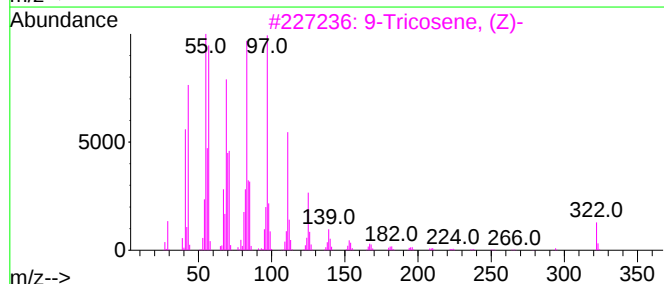
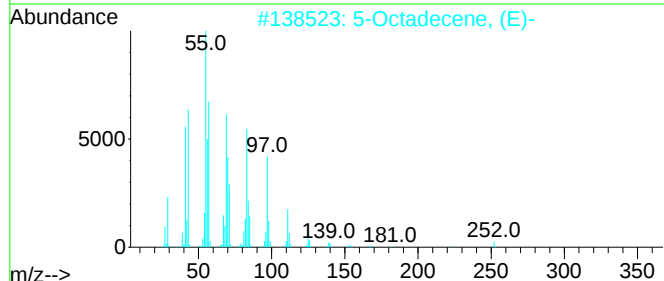
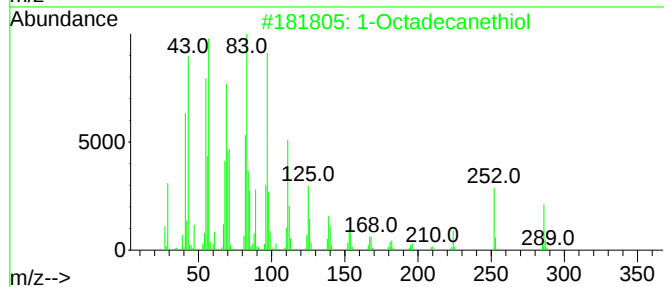
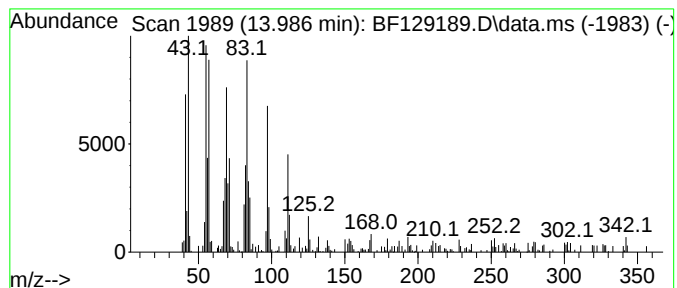
Instrument :
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ClientSampleId :
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TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Octadecanethiol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.986	5.08 ng	257391	Chrysene-d12		14.110	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1-Octadecanethiol		286	C18H38S	002885-00-9	95
2	5-Octadecene, (E)-		252	C18H36	007206-21-5	93
3	9-Tricosene, (Z)-		322	C23H46	027519-02-4	93
4	Cyclopentadecane		210	C15H30	000295-48-7	93
5	1-Tricosene		322	C23H46	018835-32-0	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071222\
Data File : BF129189.D
Acq On : 12 Jul 2022 15:05
Operator : CG\JU
Sample : N3662-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220498B-SIM/C4B-COMPOSITE

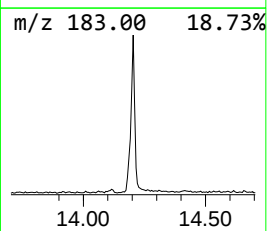
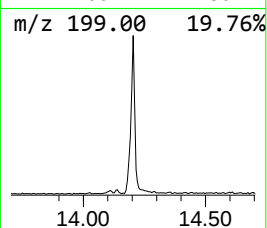
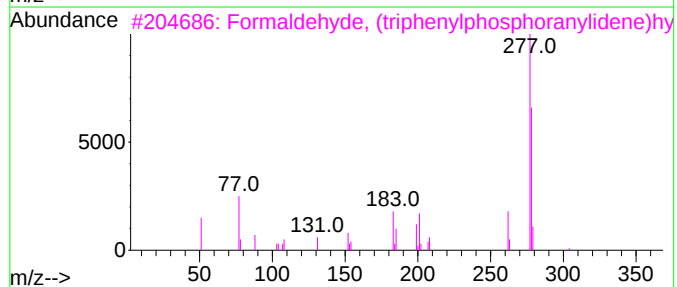
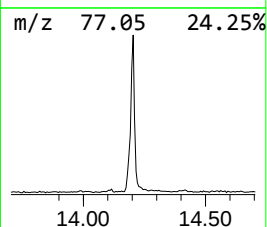
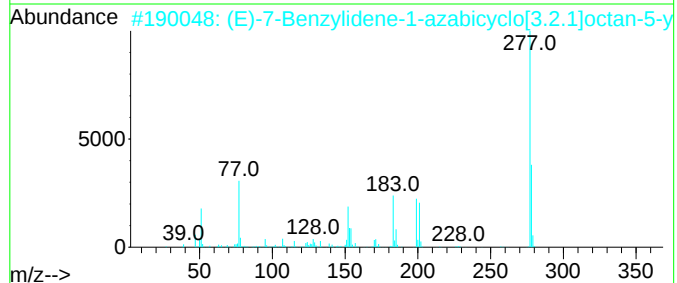
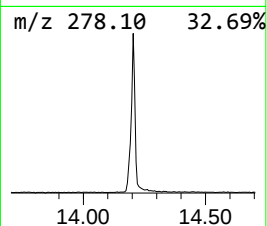
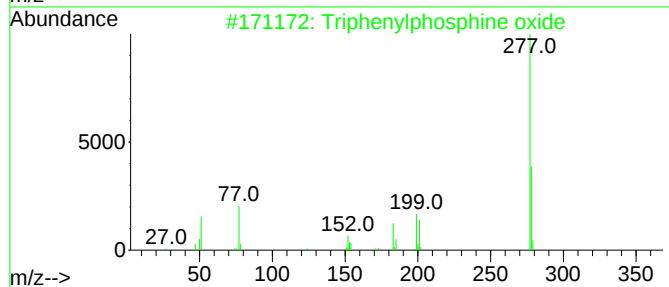
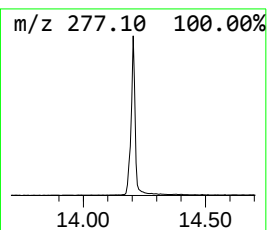
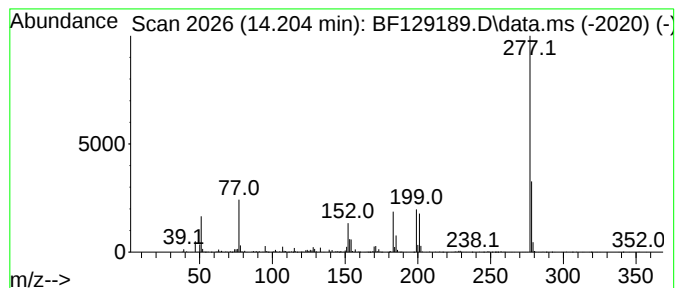
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Triphenylphosphine oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.204	14.57 ng	738228	Chrysene-d12	14.110

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	96
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	76
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	59
4			Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	28
5			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071222\
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Sample : N3662-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220498B-SIM/C4B-COMPOSITE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.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...	2.328	48.7	ng	4316500	1	6.934	1771700	20.0
Hexadecane	9.680	2.0	ng	252747	3	9.975	2463730	20.0
Pentadecane, 2,...	10.880	3.3	ng	356110	4	11.463	2193380	20.0
Octadecane	11.345	2.3	ng	247244	4	11.463	2193380	20.0
1-Octadecanethiol	13.986	5.1	ng	257391	5	14.110	1013140	20.0
Triphenylphosph...	14.204	14.6	ng	738228	5	14.110	1013140	20.0