

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110724\
 Data File : BF140279.D
 Acq On : 07 Nov 2024 17:06
 Operator : RC/JU
 Sample : P4720-01
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 JC-701-COMP-01

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-BF110524.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140279.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	5	21	rVB	1471191	1811386	37.38%	12.299%
2	5.481	572	576	588	rBV	219255	299876	6.19%	2.036%
3	6.157	686	691	699	rVB	135864	169646	3.50%	1.152%
4	6.493	743	748	759	rVV	245334	330817	6.83%	2.246%
5	6.581	759	763	768	rVB	60953	75233	1.55%	0.511%
6	6.875	808	813	819	rBV	586315	714878	14.75%	4.854%
7	7.434	902	908	918	rBV	158060	215485	4.45%	1.463%
8	8.157	1025	1031	1038	rBV	735233	908322	18.75%	6.167%
9	8.234	1039	1044	1051	rVB	45878	61367	1.27%	0.417%
10	9.228	1208	1213	1223	rBV	314109	394067	8.13%	2.676%
11	9.910	1324	1329	1339	rBV	762867	1004101	20.72%	6.818%
12	10.628	1445	1451	1458	rBV	125255	162795	3.36%	1.105%
13	10.698	1458	1463	1471	rVV	143055	188241	3.88%	1.278%
14	10.951	1500	1506	1513	rBV3	66691	101899	2.10%	0.692%
15	11.404	1577	1583	1591	rBV	673185	940019	19.40%	6.382%
16	11.933	1664	1673	1683	rBV3	211892	381318	7.87%	2.589%
17	12.016	1683	1687	1696	rVB2	28234	62957	1.30%	0.427%
18	12.616	1784	1789	1794	rBV	143480	191400	3.95%	1.300%
19	12.716	1802	1806	1810	rBV	39130	61981	1.28%	0.421%
20	12.845	1822	1828	1834	rVB	130661	192708	3.98%	1.308%
21	12.986	1845	1852	1859	rVB	245003	338637	6.99%	2.299%
22	13.174	1877	1884	1889	rBV2	19420	52814	1.09%	0.359%
23	13.904	2003	2008	2016	rBV4	54376	114651	2.37%	0.778%
24	14.033	2024	2030	2044	rBV2	3009677	4845557	100.00%	32.900%
25	14.516	2108	2112	2117	rBV4	30288	64412	1.33%	0.437%
26	15.098	2207	2211	2220	rBV	74226	176518	3.64%	1.199%
27	15.404	2260	2263	2269	rVB	35008	53181	1.10%	0.361%
28	15.468	2270	2274	2279	rVV	52564	84051	1.73%	0.571%
29	15.533	2280	2285	2296	rVB	362537	596510	12.31%	4.050%
30	16.015	2362	2367	2374	rVB	74376	133343	2.75%	0.905%

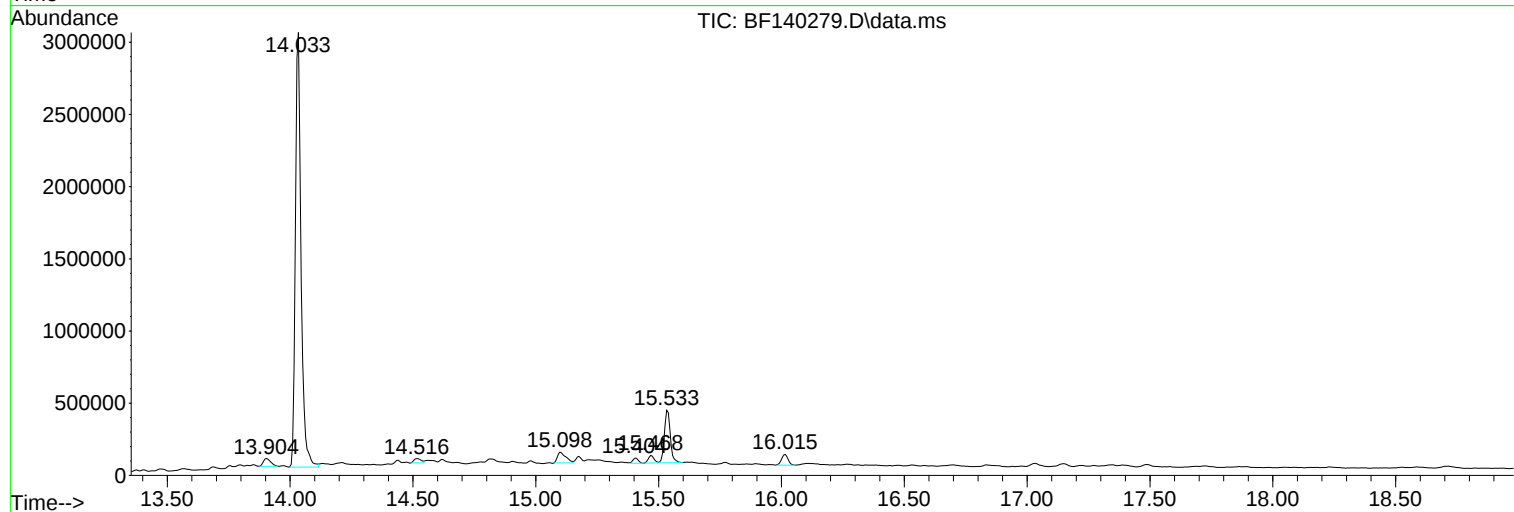
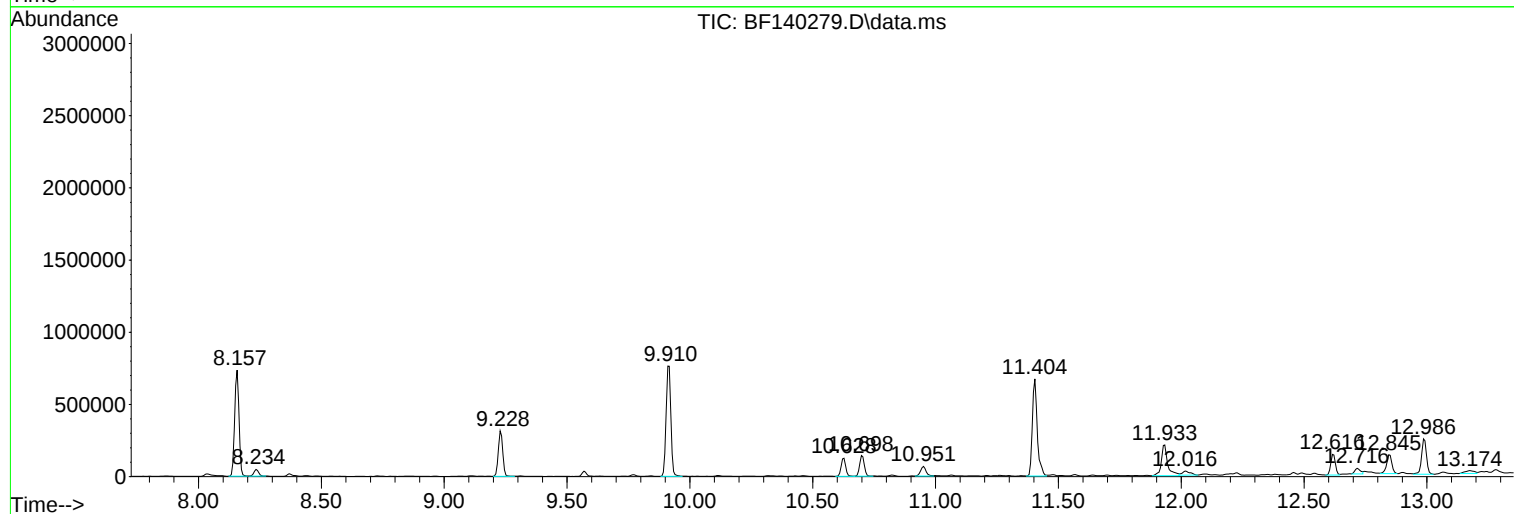
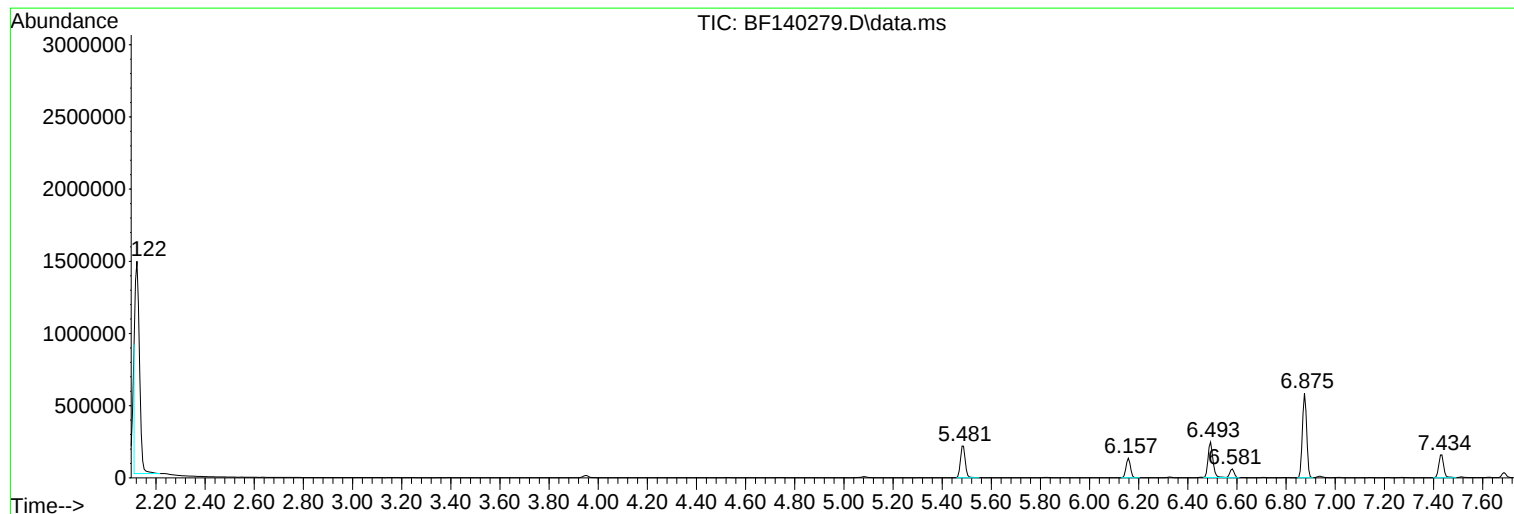
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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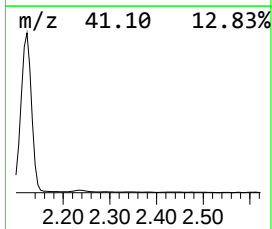
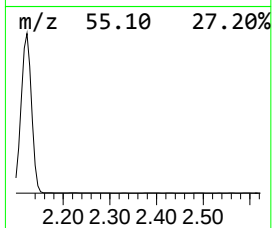
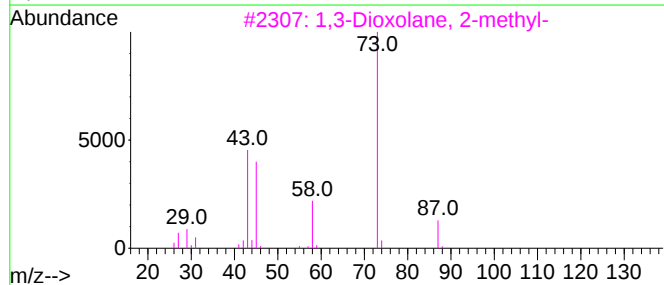
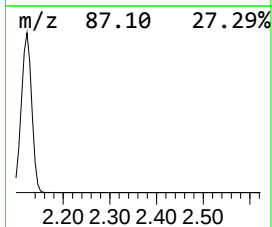
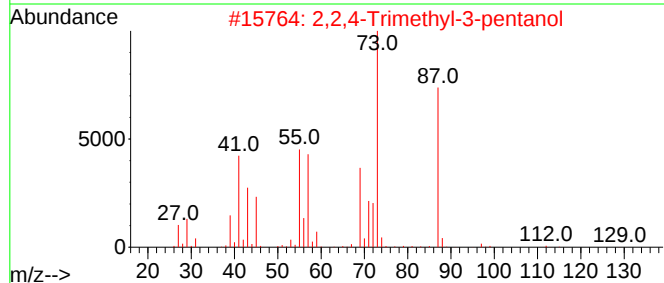
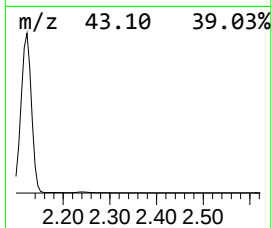
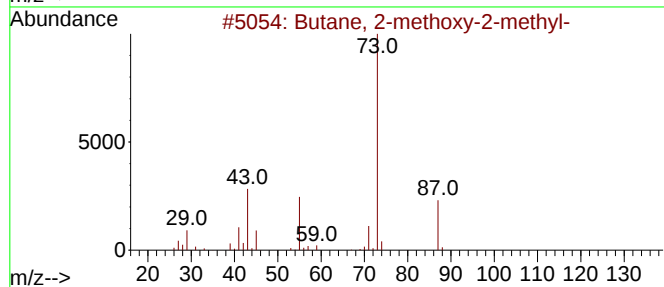
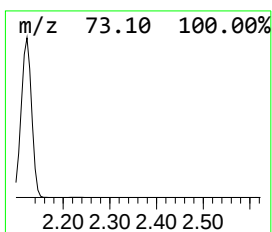
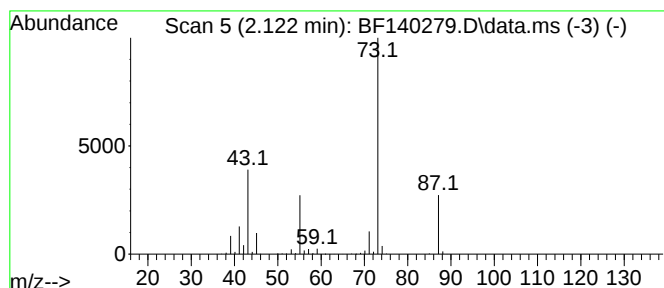
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.122	50.68 ng	1811390	1,4-Dichlorobenzene-d4	6.875

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			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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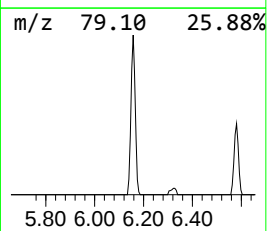
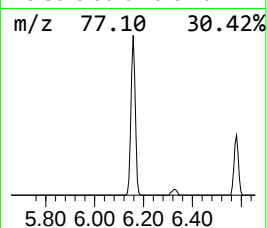
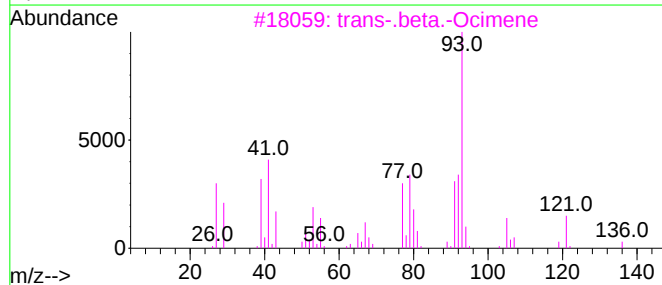
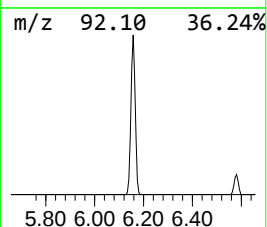
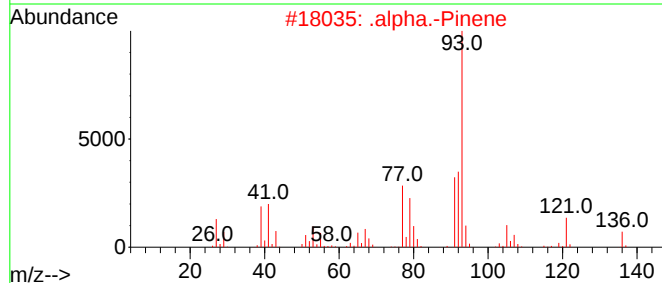
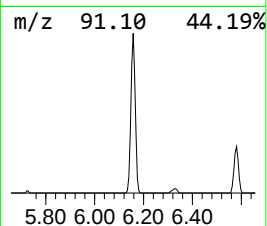
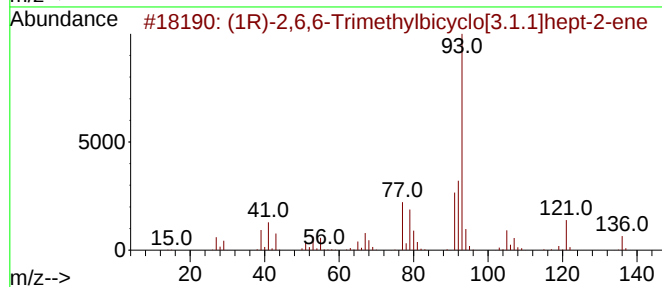
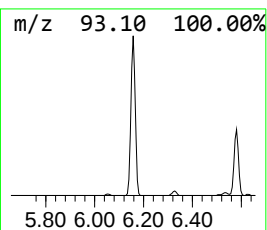
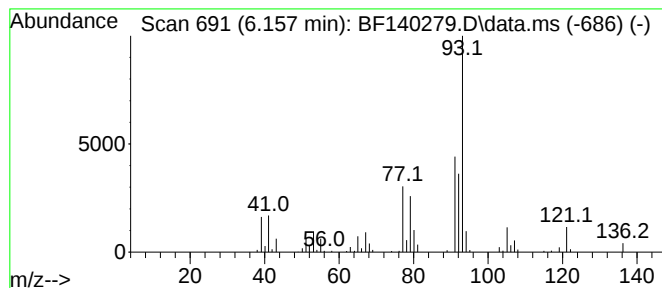
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 (1R)-2,6,6-Trimethylbicyclo... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.157	4.75 ng	169646	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(1R)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	136	C10H16	007785-70-8	95
2			.alpha.-Pinene	136	C10H16	000080-56-8	94
3			trans-.beta.-Ocimene	136	C10H16	003779-61-1	94
4			Bicyclo[3.1.1]hept-2-ene, 3,6,6-trimethyl-	136	C10H16	004889-83-2	91
5			Tricyclo[2.2.1.0(2,6)]heptane, 1,1,1-trimethyl-	136	C10H16	000508-32-7	91



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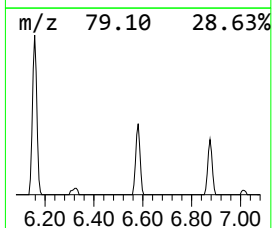
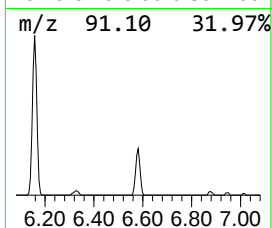
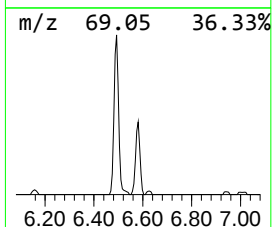
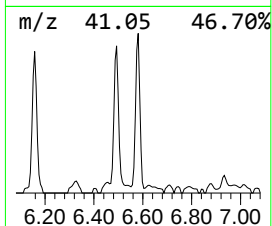
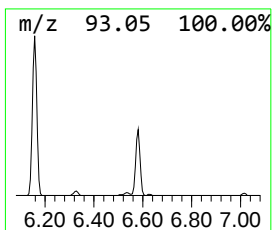
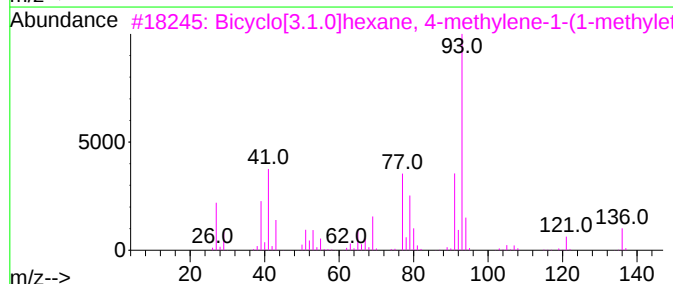
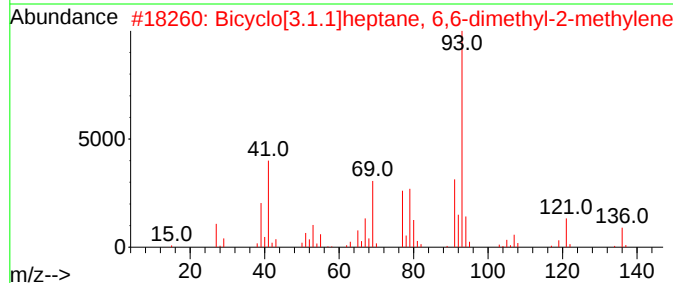
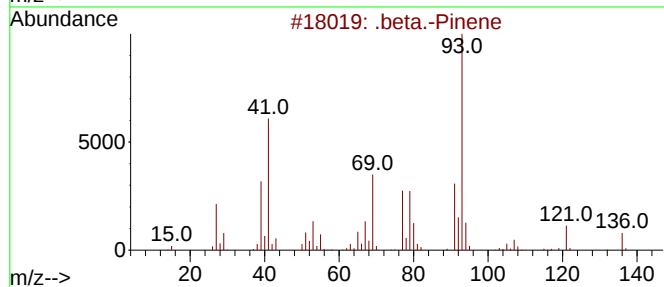
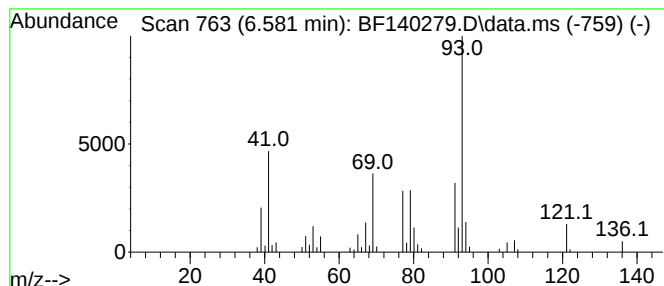
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 .beta.-Pinene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.581	2.10 ng	75233	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.	.beta.-Pinene	136	C10H16	000127-91-3	95	
2	Bicyclo[3.1.1]heptane, 6,6-dimet...	136	C10H16	018172-67-3	94		
3	Bicyclo[3.1.0]hexane, 4-methylen...	136	C10H16	003387-41-5	87		
4	Cyclohexene, 4-methylene-1-(1-me...	136	C10H16	000099-84-3	83		
5	.beta.-Myrcene	136	C10H16	000123-35-3	80		



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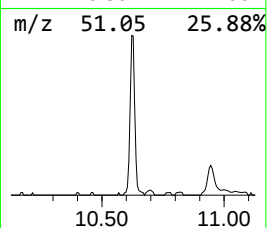
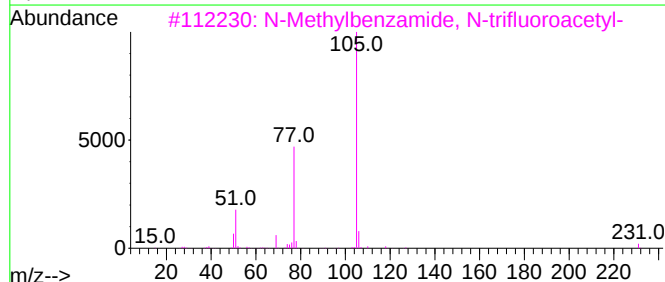
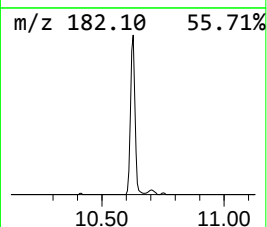
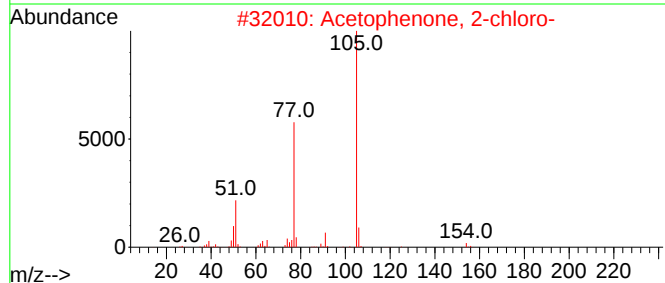
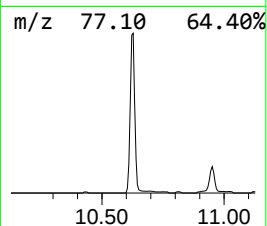
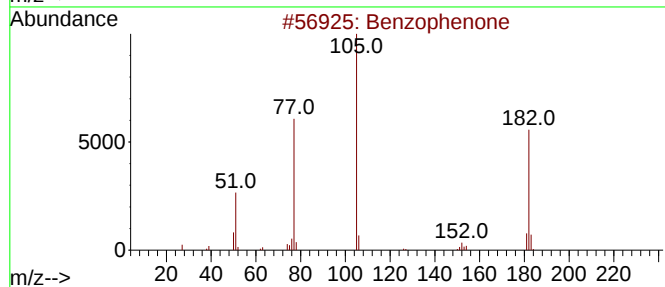
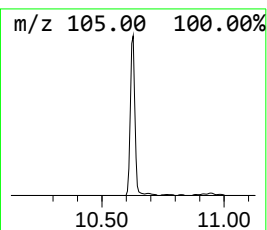
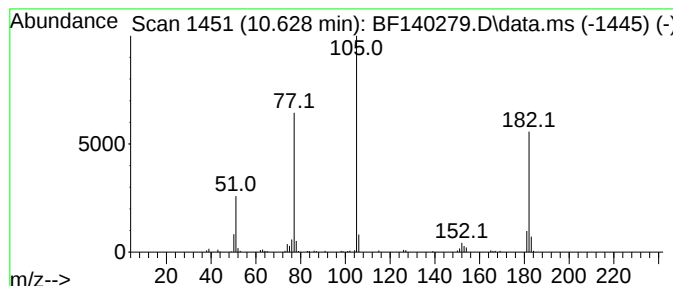
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Peak Number 4 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.628	3.24 ng	162795	Acenaphthene-d10	9.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47
4			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47
5			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47



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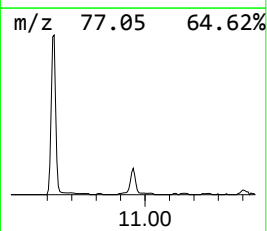
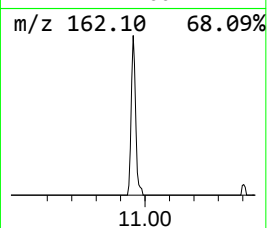
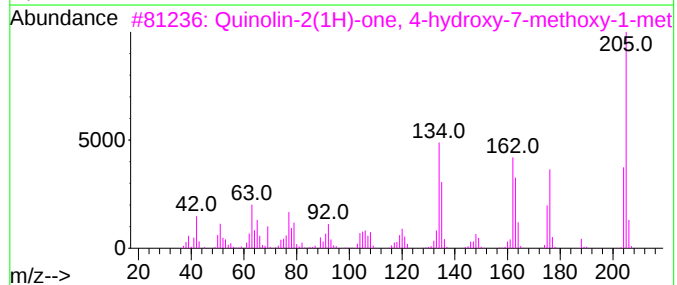
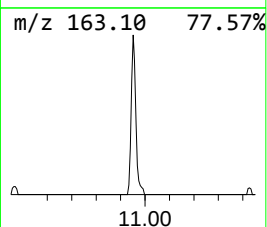
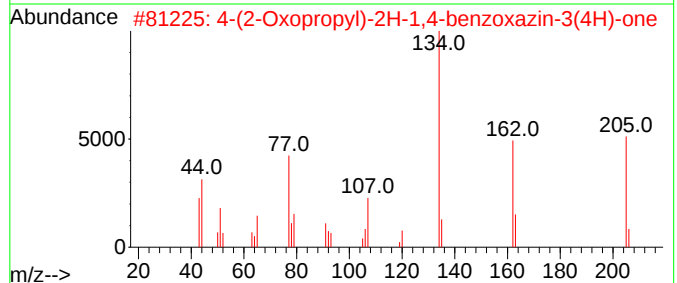
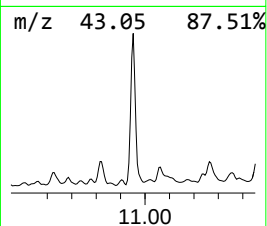
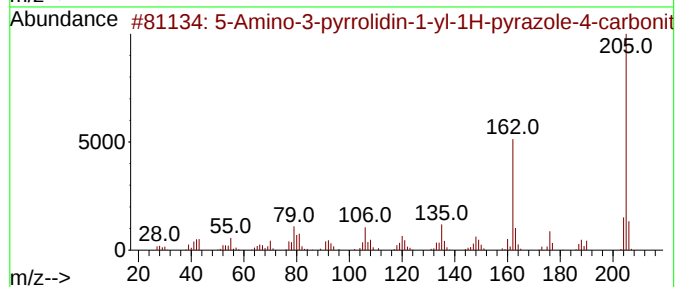
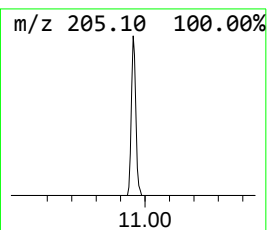
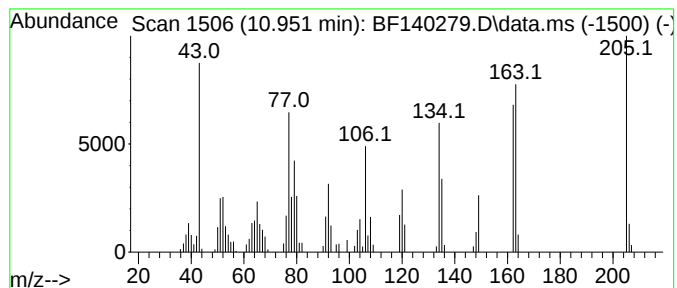
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 unknown10.951 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.951	2.17 ng	101899	Phenanthrene-d10	11.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Amino-3-pyrrolidin-1-yl-1H-pyr...	205	C10H15N5	1000499-90-2	43
2			4-(2-Oxopropyl)-2H-1,4-benzoxazi...	205	C11H11NO3	105492-42-0	38
3			Quinolin-2(1H)-one, 4-hydroxy-7-...	205	C11H11NO3	074798-86-0	30
4			1H-isoindole-1,3(2H)-dione, 5-hy...	163	C8H5NO3	1000404-43-3	25
5			1H-Pyrazolo[3,4-b]pyridin-3-ylamine	134	C6H6N4	1000303-41-7	25



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ALS Vial : 20 Sample Multiplier: 1

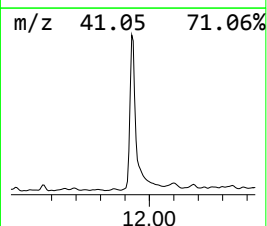
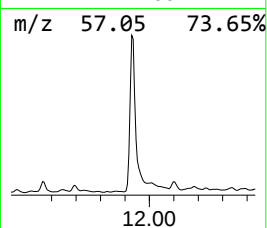
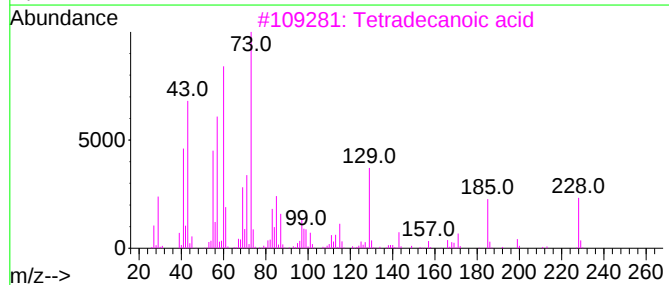
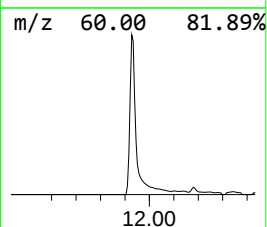
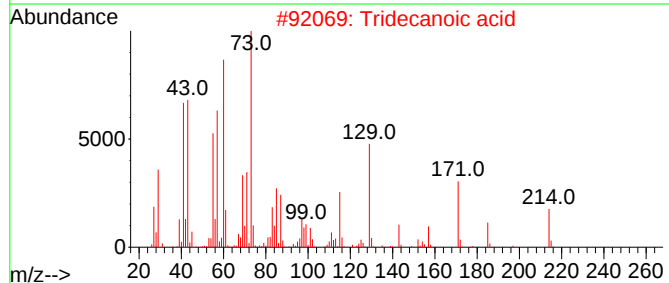
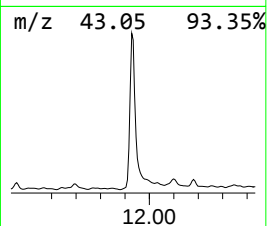
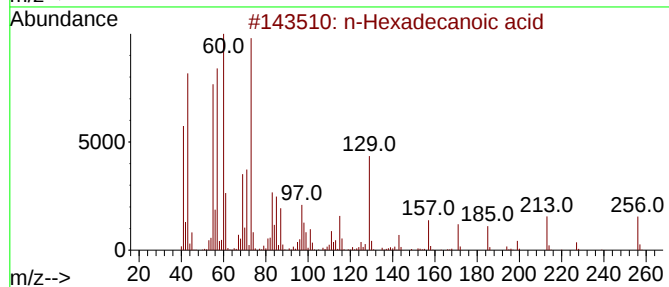
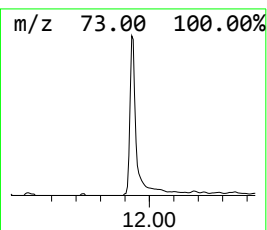
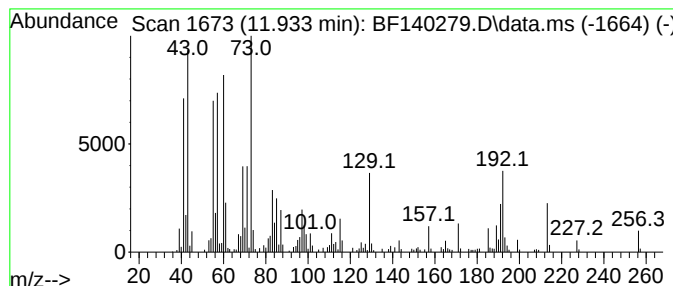
Instrument :
BNA_F
ClientSampleId :
JC-701-COMP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.933	8.11 ng	381318	Phenanthrene-d10	11.404	
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	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110724\
Data File : BF140279.D
Acq On : 07 Nov 2024 17:06
Operator : RC/JU
Sample : P4720-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

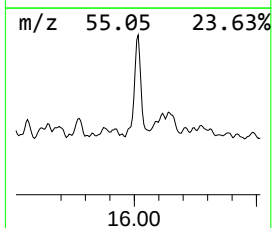
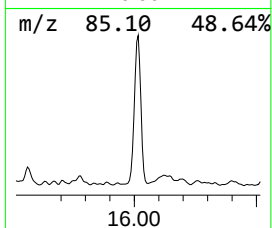
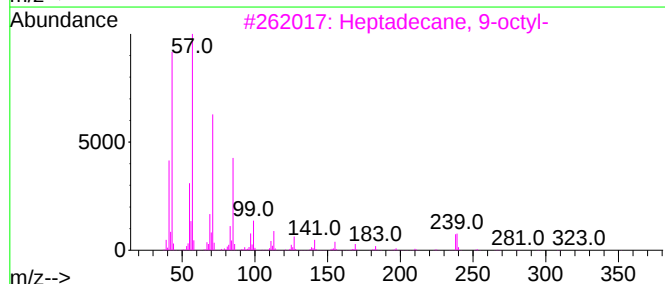
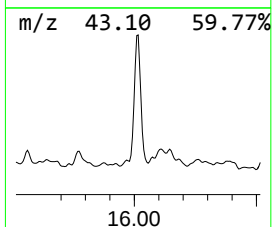
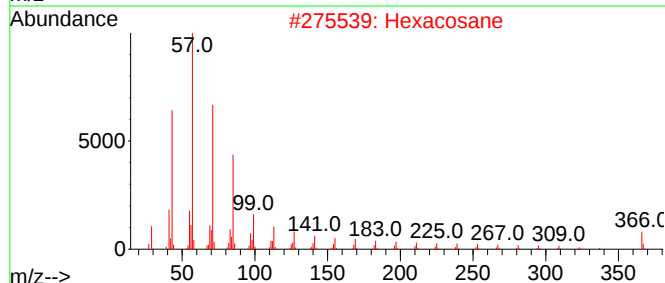
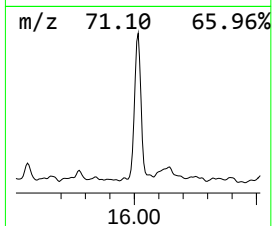
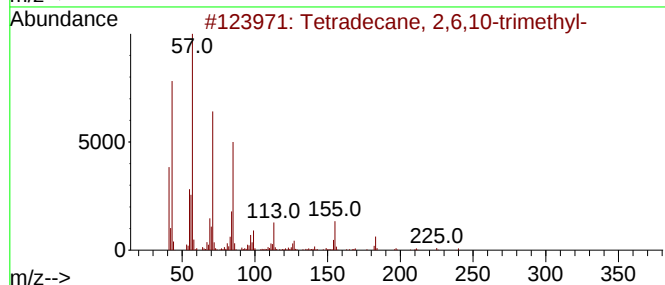
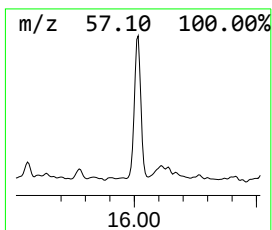
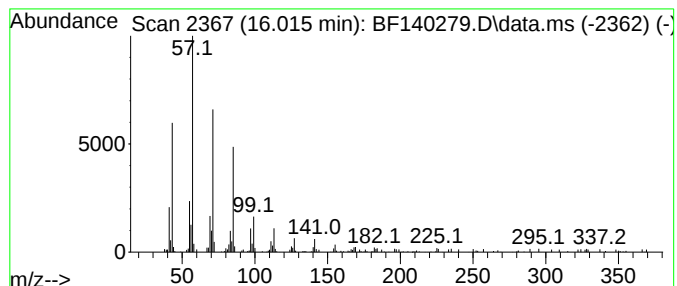
Instrument :
BNA_F
ClientSampleId :
JC-701-COMP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetradecane, 2,6,10-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.015	4.47 ng	133343	Perylene-d12	15.533	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	93
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
4	Octacosane	394	C28H58	000630-02-4	90
5	Heneicosane	296	C21H44	000629-94-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110724\
Data File : BF140279.D
Acq On : 07 Nov 2024 17:06
Operator : RC/JU
Sample : P4720-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
JC-701-COMP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.122	50.7	ng	1811390	1	6.875	714878	20.0
(1R)-2,6,6-Trim...	6.157	4.8	ng	169646	1	6.875	714878	20.0
.beta.-Pinene	6.581	2.1	ng	75233	1	6.875	714878	20.0
Benzophenone	10.628	3.2	ng	162795	3	9.916	1004100	20.0
unknown10.951	10.951	2.2	ng	101899	4	11.404	940019	20.0
n-Hexadecanoic ...	11.933	8.1	ng	381318	4	11.404	940019	20.0
Tetradecane, 2,...	16.015	4.5	ng	133343	6	15.533	596510	20.0