

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111924\
 Data File : BF140486.D
 Acq On : 19 Nov 2024 20:47
 Operator : RC/JU
 Sample : P4768-07
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-6-3

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-BF111324.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140486.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	4	12	22	rVB	1532930	2405312	87.12%	11.100%
2	2.269	24	30	39	rVB3	48847	84146	3.05%	0.388%
3	5.098	505	511	522	rVB	89113	135421	4.91%	0.625%
4	5.469	569	574	575	rBV	60067	65817	2.38%	0.304%
5	5.504	575	580	590	rVB	1788271	2430828	88.05%	11.218%
6	5.728	614	618	623	rVB	25728	33417	1.21%	0.154%
7	6.510	745	751	764	rBV	1826654	2491200	90.24%	11.497%
8	6.704	779	784	795	rVB2	32197	47115	1.71%	0.217%
9	6.875	808	813	818	rVB	603389	743247	26.92%	3.430%
10	7.434	902	908	917	rBV	1198315	1568807	56.82%	7.240%
11	7.686	945	951	962	rVB	27871	43648	1.58%	0.201%
12	8.151	1022	1030	1048	rBV	684152	927405	33.59%	4.280%
13	9.228	1207	1213	1223	rBV	2136758	2760780	100.00%	12.741%
14	9.910	1323	1329	1343	rBV	652736	867372	31.42%	4.003%
15	10.622	1444	1450	1458	rBV	385929	498027	18.04%	2.298%
16	10.698	1458	1463	1473	rBV	999329	1317738	47.73%	6.081%
17	10.933	1498	1503	1509	rVB	36526	51502	1.87%	0.238%
18	11.398	1577	1582	1591	rBV	628438	865251	31.34%	3.993%
19	11.921	1665	1671	1683	rVV2	227677	410659	14.87%	1.895%
20	12.010	1683	1686	1695	rVB3	21834	47221	1.71%	0.218%
21	12.616	1785	1789	1794	rBV	59117	83878	3.04%	0.387%
22	12.710	1801	1805	1812	rBV4	27775	52275	1.89%	0.241%
23	12.845	1823	1828	1834	rBV	55673	84010	3.04%	0.388%
24	12.980	1846	1851	1859	rBV	1674404	2262356	81.95%	10.441%
25	13.463	1928	1933	1940	rVB	121198	173945	6.30%	0.803%
26	14.045	2027	2032	2040	rBV	425012	613237	22.21%	2.830%
27	14.886	2172	2175	2181	rVB	114181	153920	5.58%	0.710%
28	15.533	2280	2285	2292	rVB	272843	450360	16.31%	2.078%

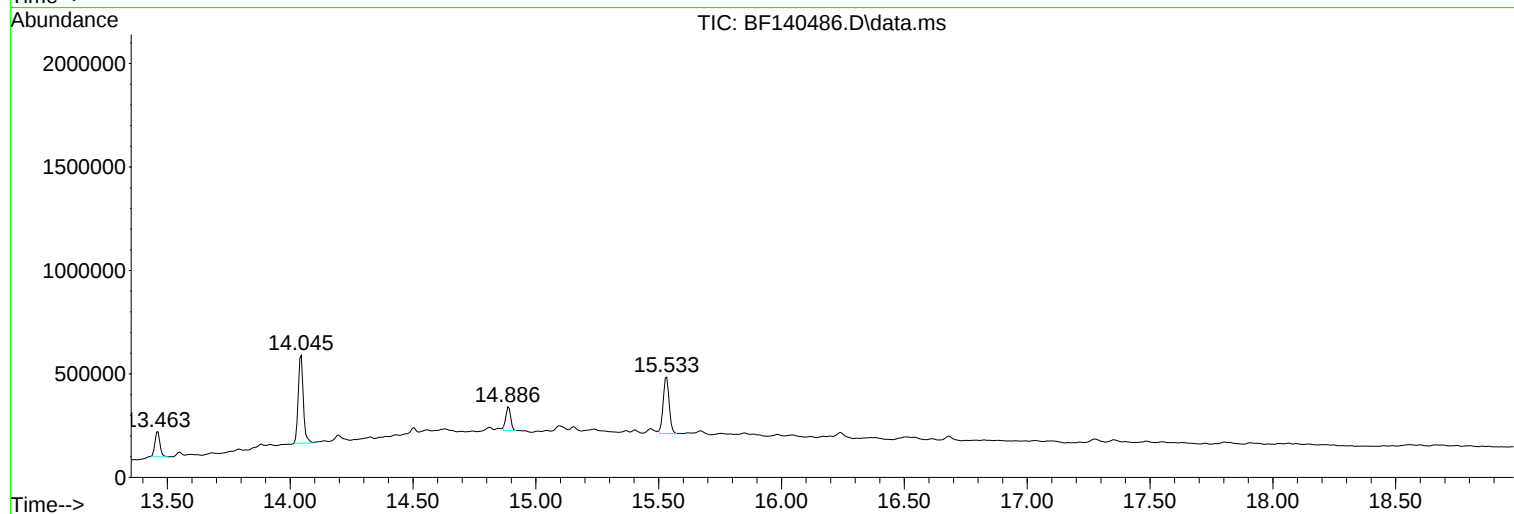
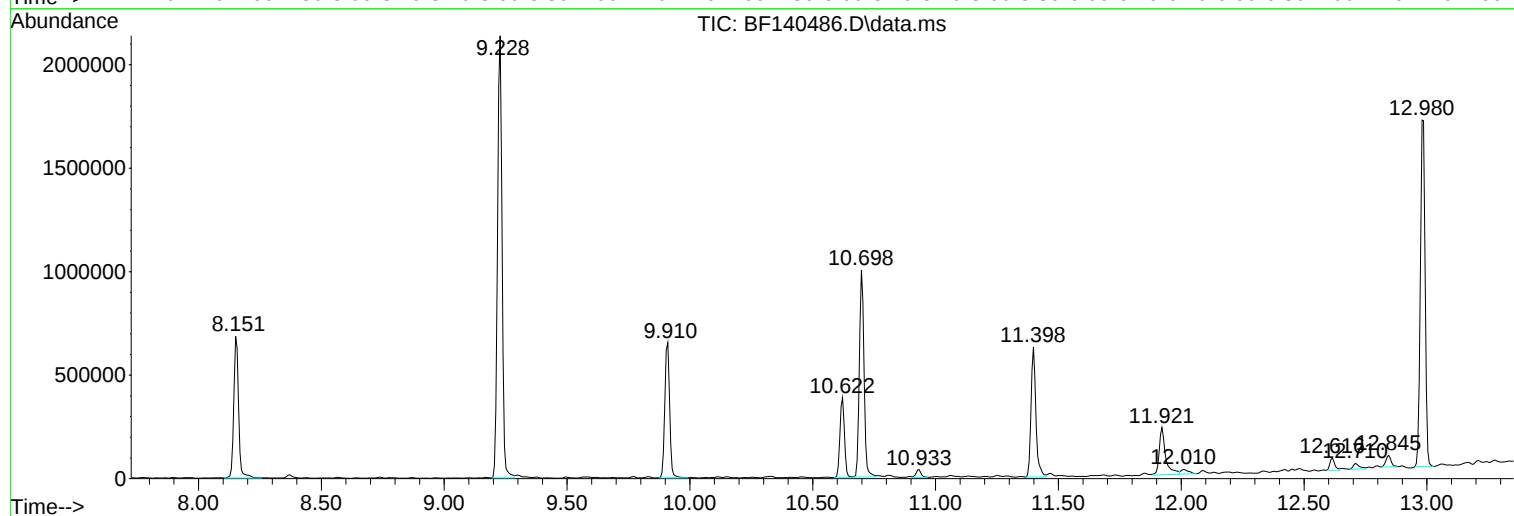
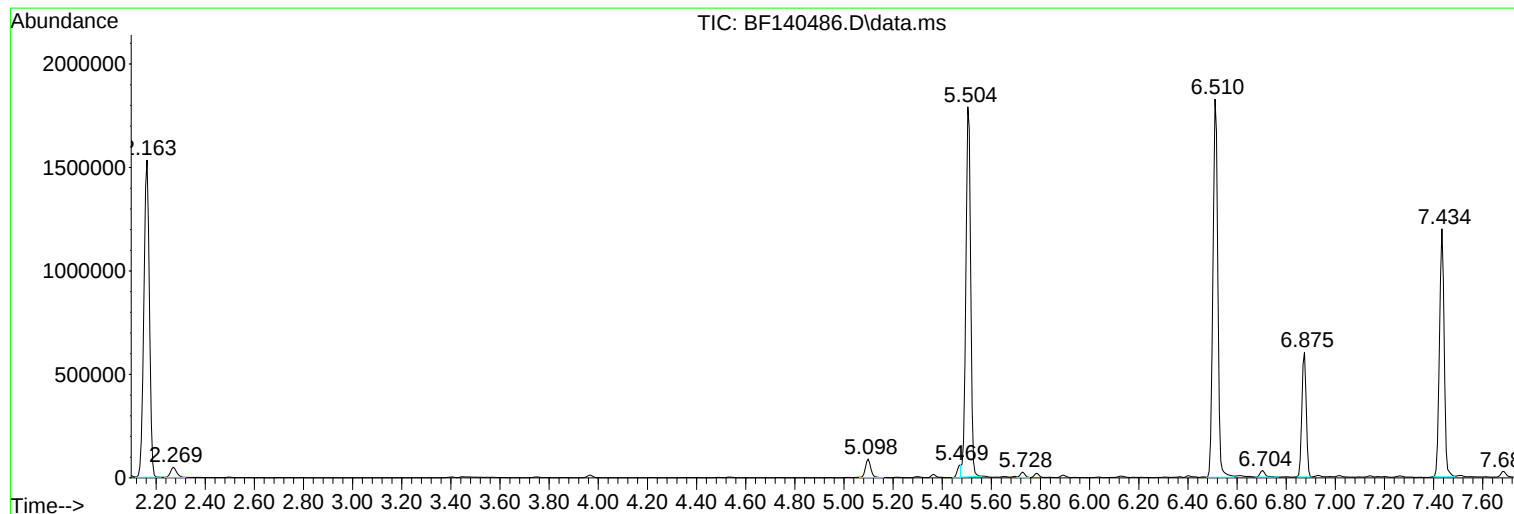
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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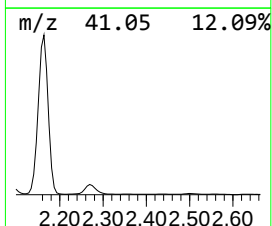
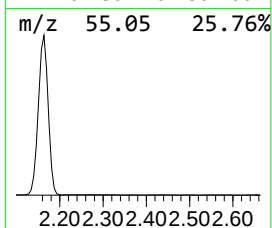
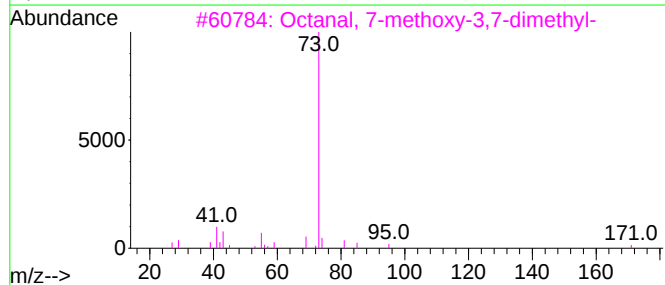
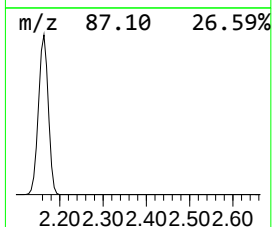
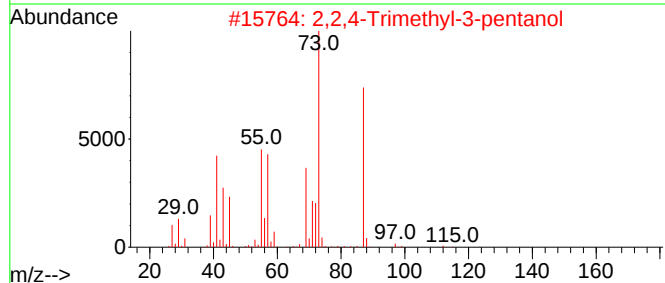
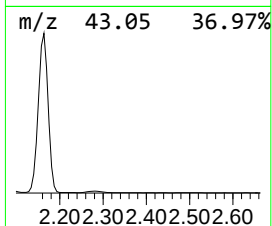
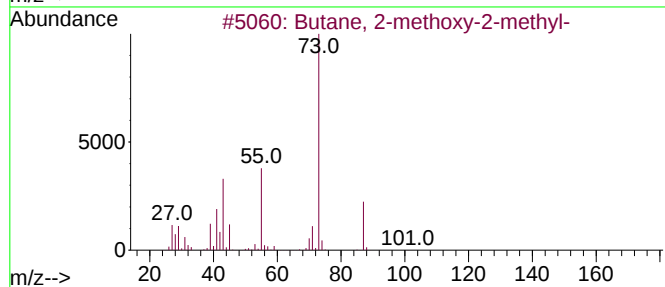
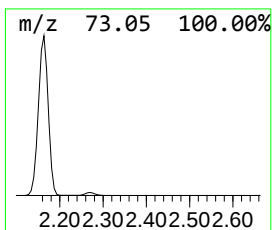
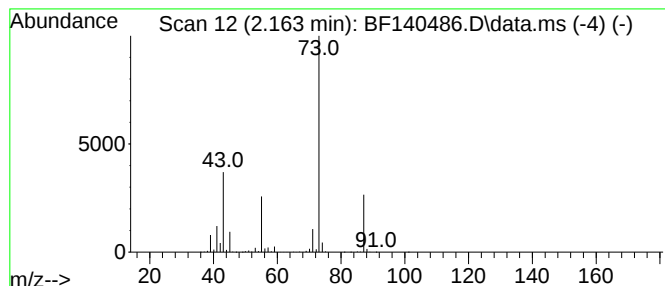
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.163	64.72 ng	2405310	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	40
3			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	23
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17



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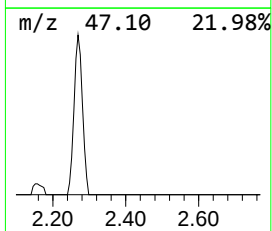
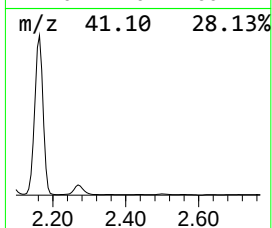
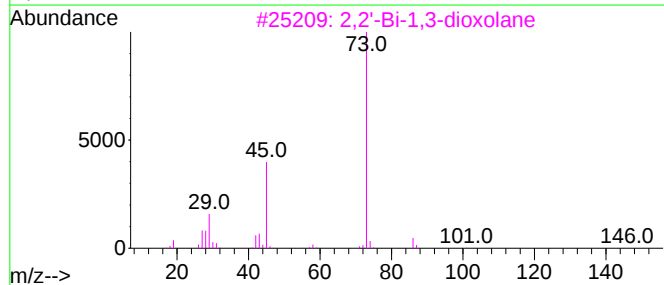
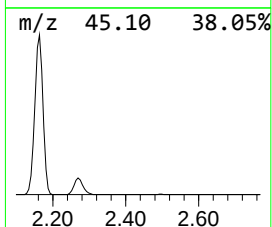
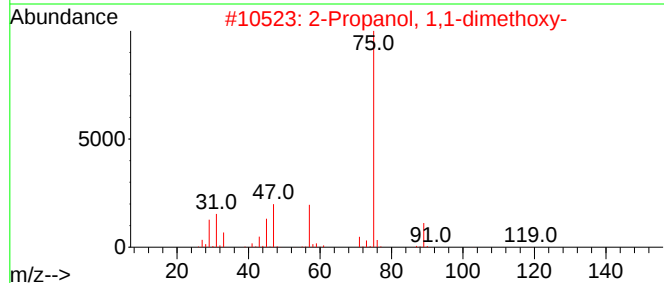
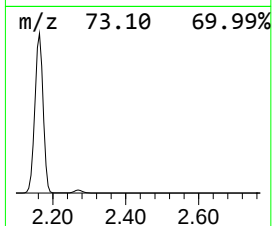
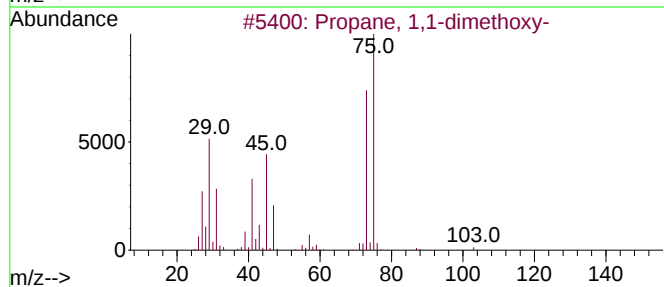
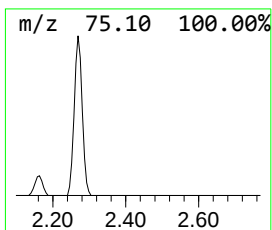
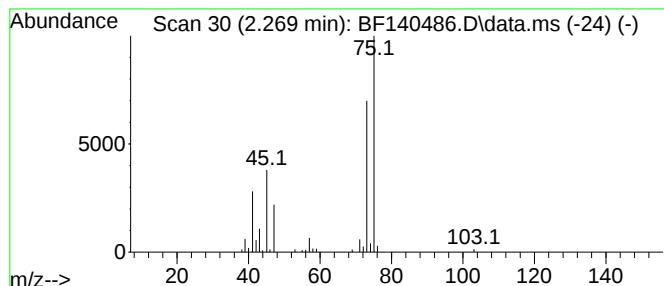
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.269	2.26 ng	84146	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2			2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	36
3			2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	14
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5			2,5-Diethoxy-3-methyl-3-vinylhexane	214	C13H26O2	1000432-70-8	10



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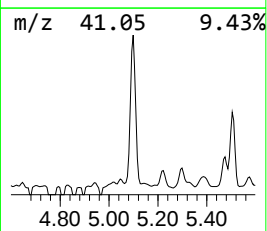
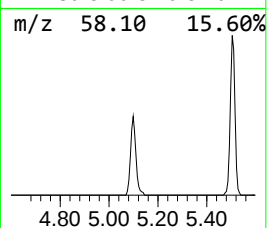
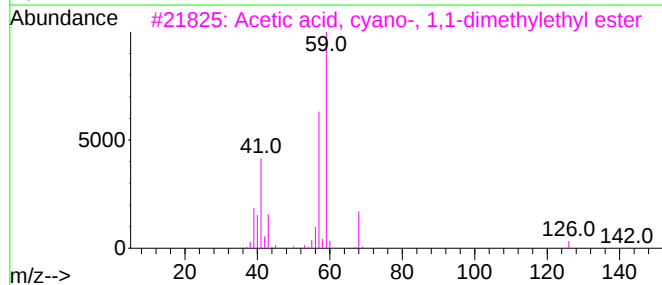
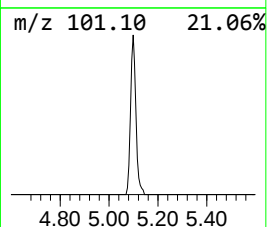
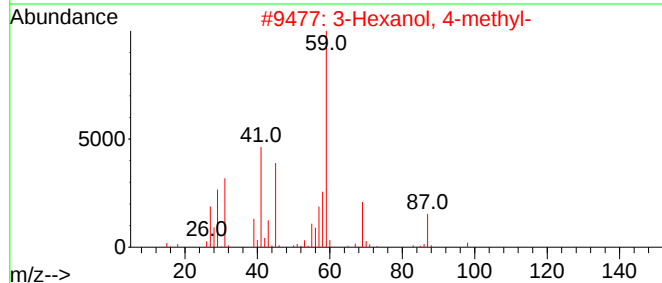
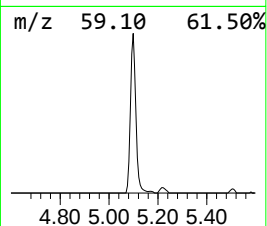
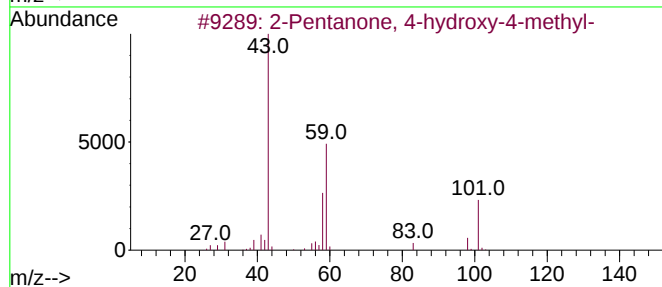
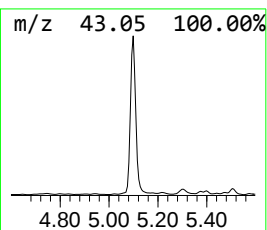
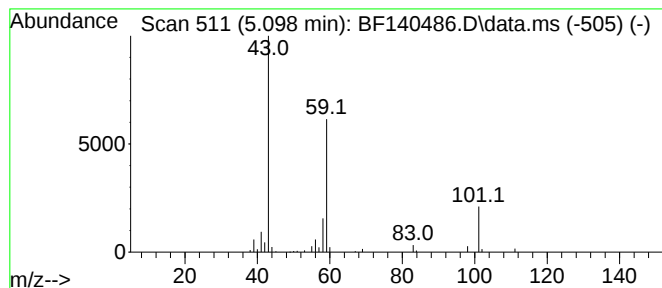
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.098	3.64 ng	135421	1,4-Dichlorobenzene-d4	6.875

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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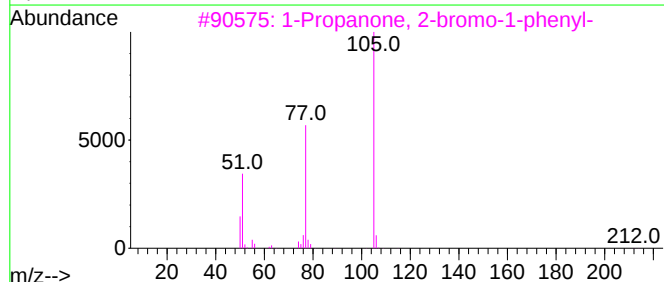
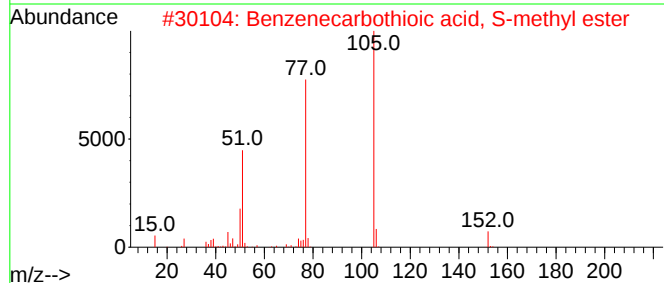
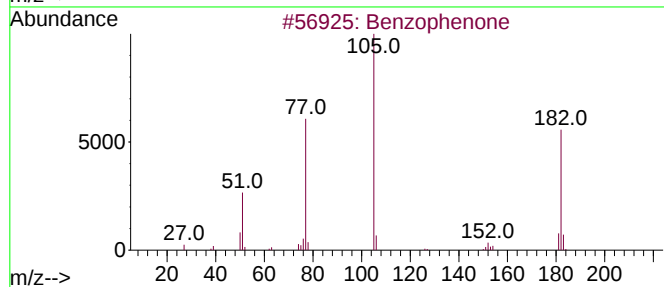
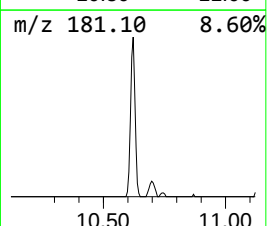
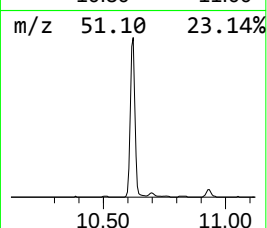
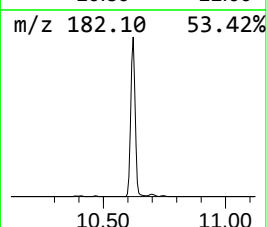
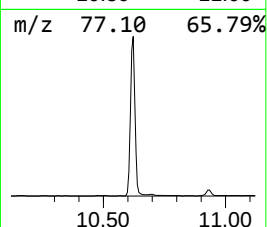
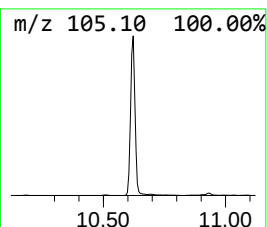
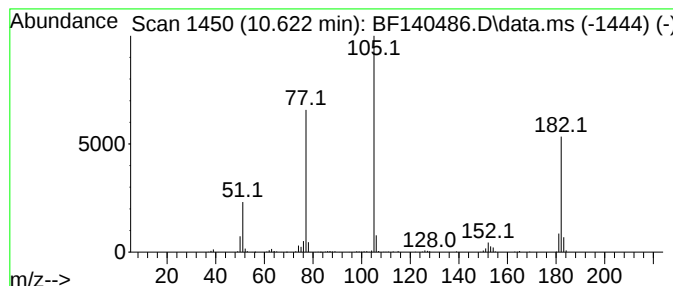
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Peak Number 4 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.622	11.48 ng	498027	Acenaphthene-d10	9.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	50
3			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
4			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
5			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47



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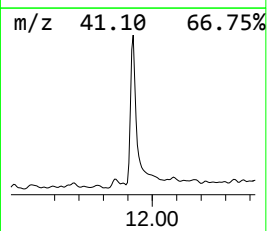
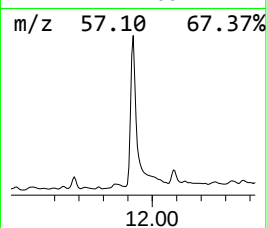
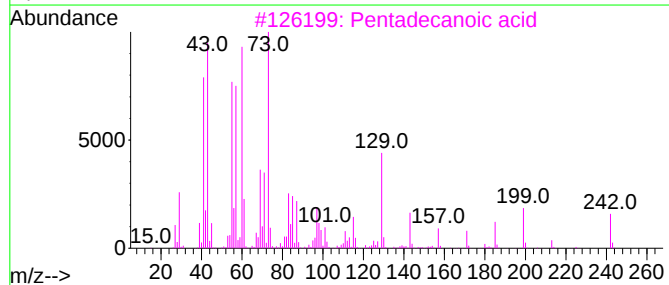
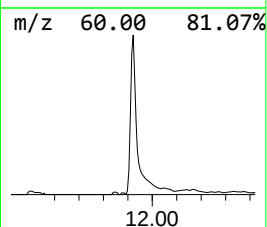
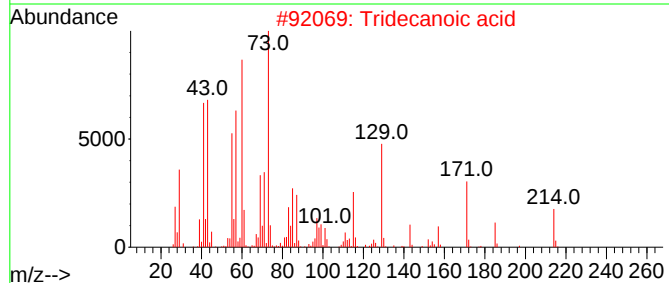
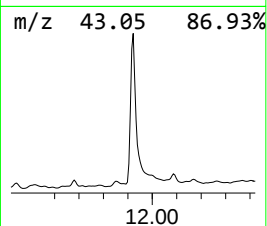
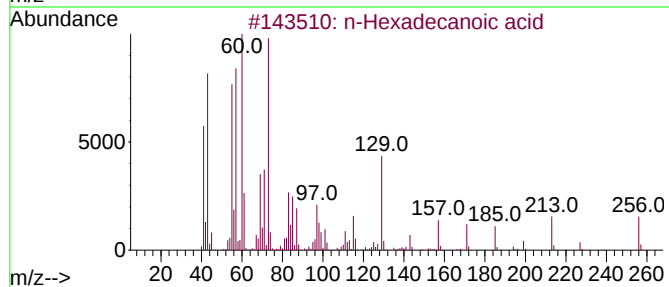
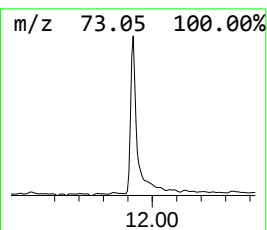
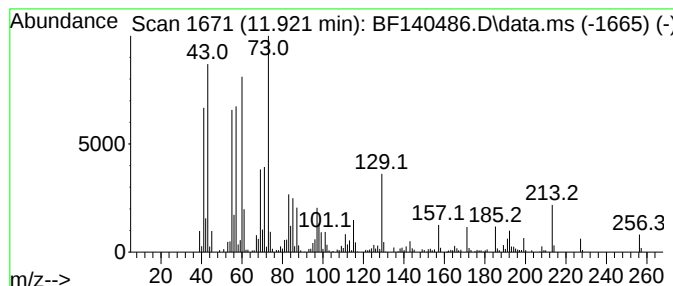
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	9.49 ng	410659	Phenanthrene-d10	11.398

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	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60



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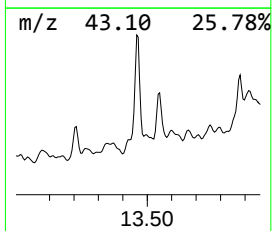
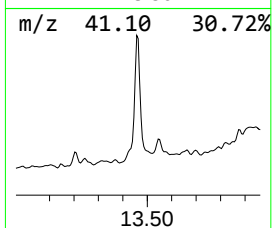
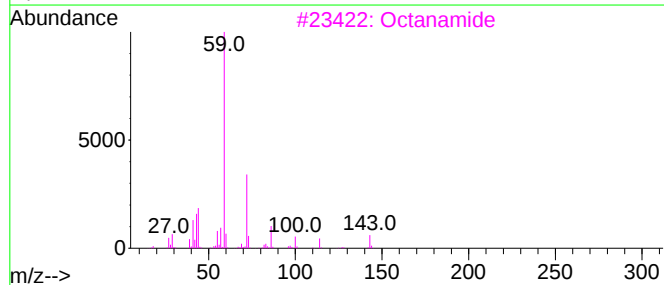
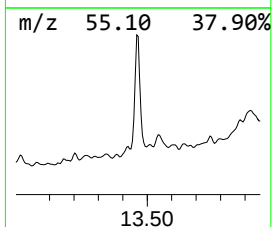
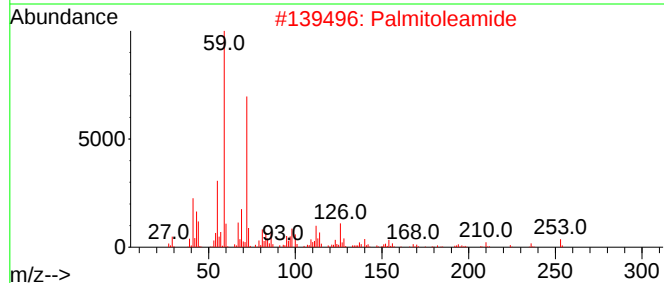
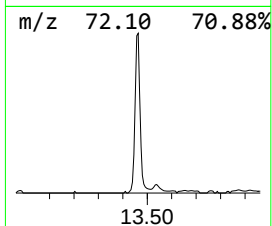
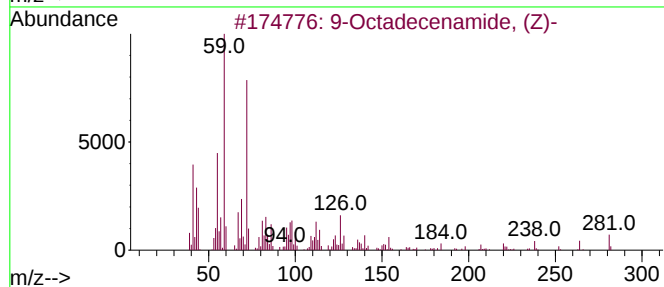
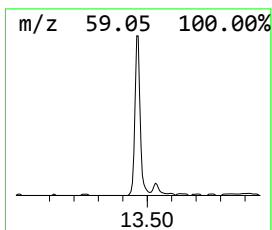
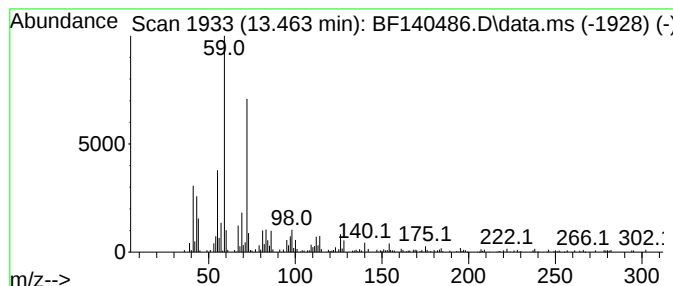
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.463	5.67 ng	173945	Chrysene-d12	14.045

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	94
2		Palmitoleamide	253	C16H31NO	106010-22-4	83
3		Octanamide	143	C8H17NO	000629-01-6	59
4		Octadecanamide	283	C18H37NO	000124-26-5	59
5		Nonanamide	157	C9H19NO	001120-07-6	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111924\
Data File : BF140486.D
Acq On : 19 Nov 2024 20:47
Operator : RC/JU
Sample : P4768-07
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-6-3

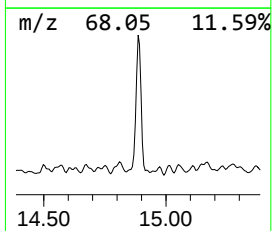
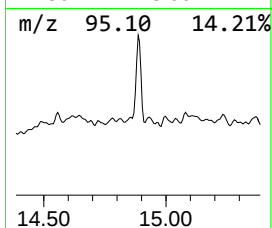
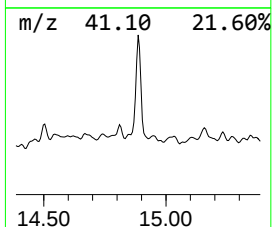
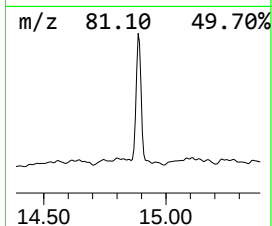
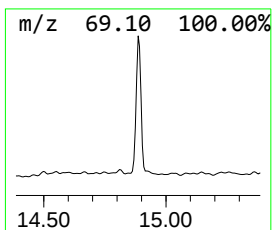
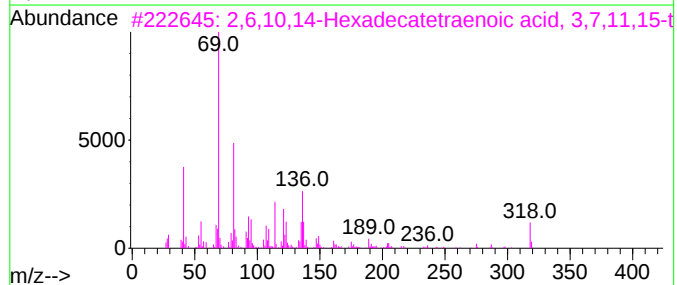
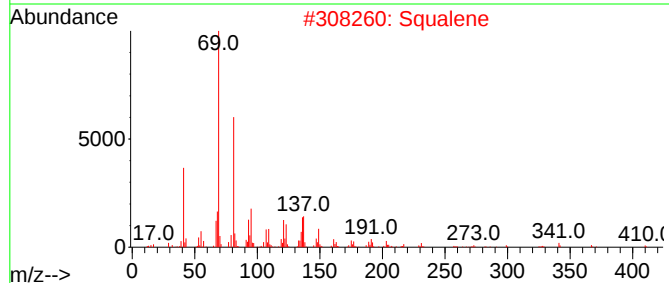
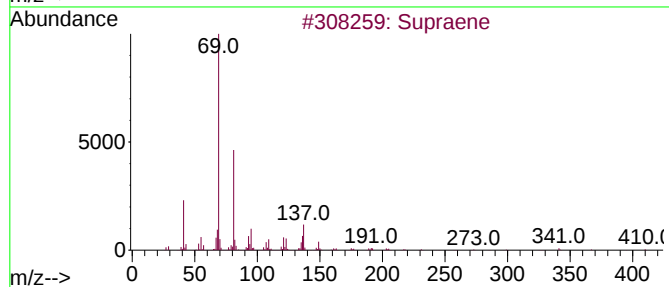
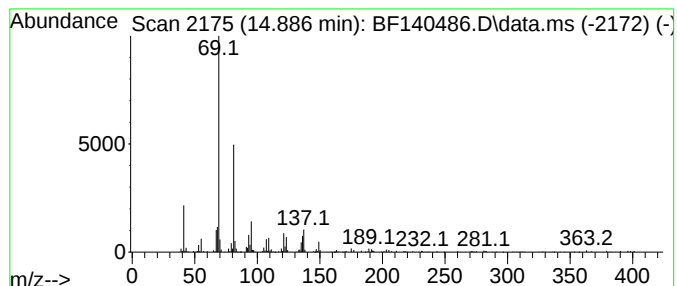
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.886	6.84 ng	153920	Perylene-d12	15.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			Squalene	410	C30H50	000111-02-4	90
3			2,6,10,14-Hexadecatetraenoic aci...	318	C21H34O2	042207-88-5	72
4			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111924\
Data File : BF140486.D
Acq On : 19 Nov 2024 20:47
Operator : RC/JU
Sample : P4768-07
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-6-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.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...	2.163	64.7	ng	2405310	1	6.875	743247	20.0
Propane, 1,1-di...	2.269	2.3	ng	84146	1	6.875	743247	20.0
2-Pentanone, 4-...	5.098	3.6	ng	135421	1	6.875	743247	20.0
Benzophenone	10.622	11.5	ng	498027	3	9.910	867372	20.0
n-Hexadecanoic ...	11.922	9.5	ng	410659	4	11.398	865251	20.0
9-Octadecenamid...	13.463	5.7	ng	173945	5	14.045	613237	20.0
Supraene	14.886	6.8	ng	153920	6	15.533	450360	20.0