

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111424\
 Data File : BF140388.D
 Acq On : 15 Nov 2024 02:42
 Operator : RC/JU
 Sample : P4789-01
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BP-F21

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: BF140388.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	3	8	16	rVB	694133	1080313	47.54%	6.292%
2	2.252	22	27	43	rVB2	38199	79245	3.49%	0.462%
3	5.093	505	510	518	rVB	145527	205136	9.03%	1.195%
4	5.516	576	582	589	rBV	1638959	2100495	92.44%	12.234%
5	5.893	641	646	652	rBV3	22005	33260	1.46%	0.194%
6	6.528	748	754	767	rBV	1627032	2225813	97.96%	12.964%
7	6.875	808	813	819	rBV	568118	718127	31.60%	4.183%
8	7.440	898	909	918	rBV	1031335	1397638	61.51%	8.140%
9	7.687	947	951	959	rVB	52408	65889	2.90%	0.384%
10	8.157	1023	1031	1038	rBV	686337	871551	38.36%	5.076%
11	9.228	1208	1213	1223	rBV	1769736	2272218	100.00%	13.234%
12	9.910	1324	1329	1338	rVB	625484	810176	35.66%	4.719%
13	10.622	1446	1450	1457	rBV	116454	148969	6.56%	0.868%
14	10.704	1459	1464	1478	rVV	853564	1095232	48.20%	6.379%
15	10.816	1479	1483	1488	rVB3	16986	28150	1.24%	0.164%
16	11.404	1578	1583	1590	rBV	599755	765574	33.69%	4.459%
17	11.469	1591	1594	1597	rVB2	21139	24000	1.06%	0.140%
18	11.928	1667	1672	1684	rBV2	137892	264366	11.63%	1.540%
19	12.092	1697	1700	1705	rBV2	21876	31279	1.38%	0.182%
20	12.645	1787	1794	1801	rBV5	95239	281521	12.39%	1.640%
21	12.986	1847	1852	1858	rBV	1367095	1770652	77.93%	10.313%
22	14.051	2029	2033	2038	rVB	371328	476421	20.97%	2.775%
23	15.539	2282	2286	2294	rVB	254242	423193	18.62%	2.465%

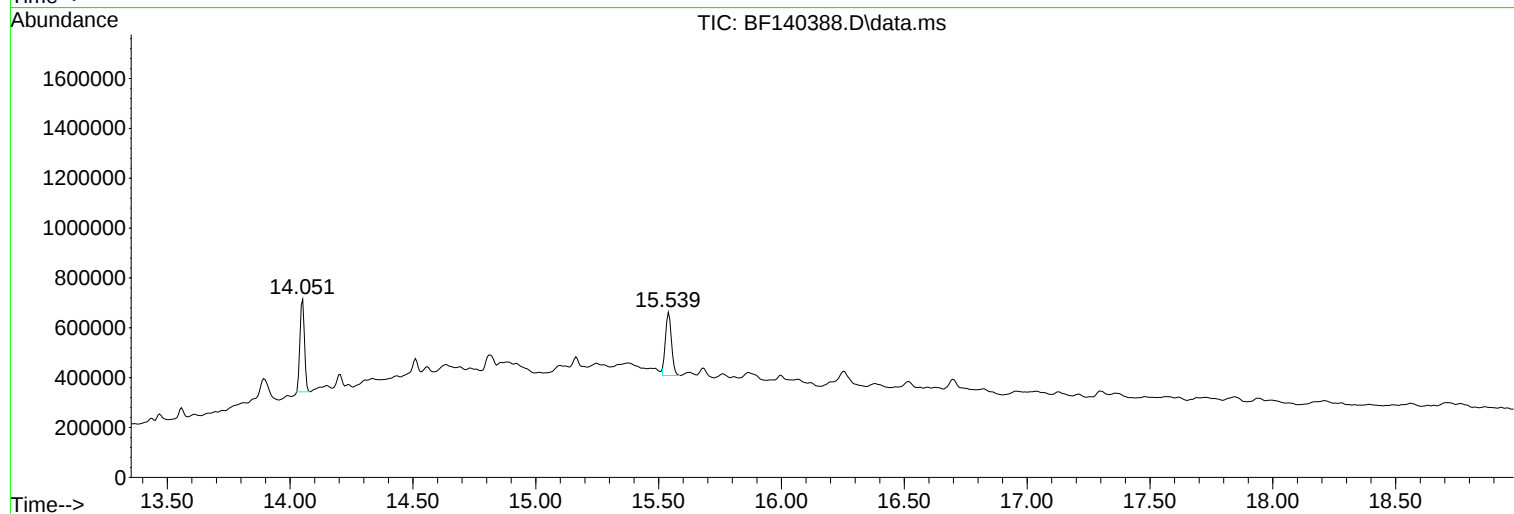
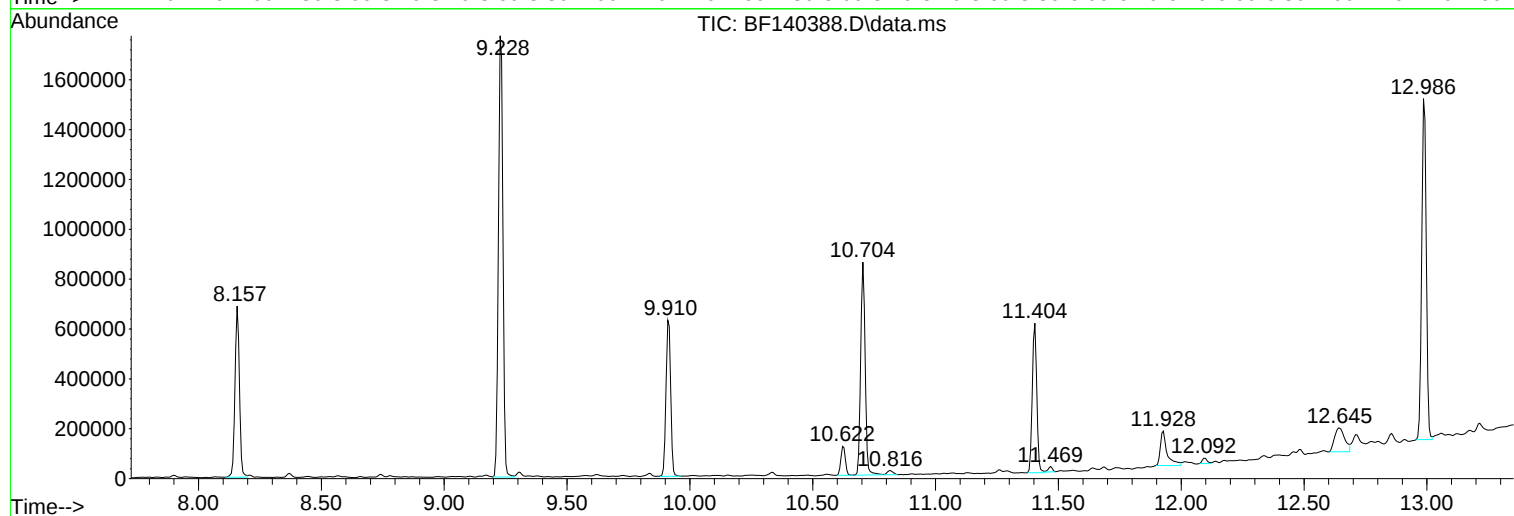
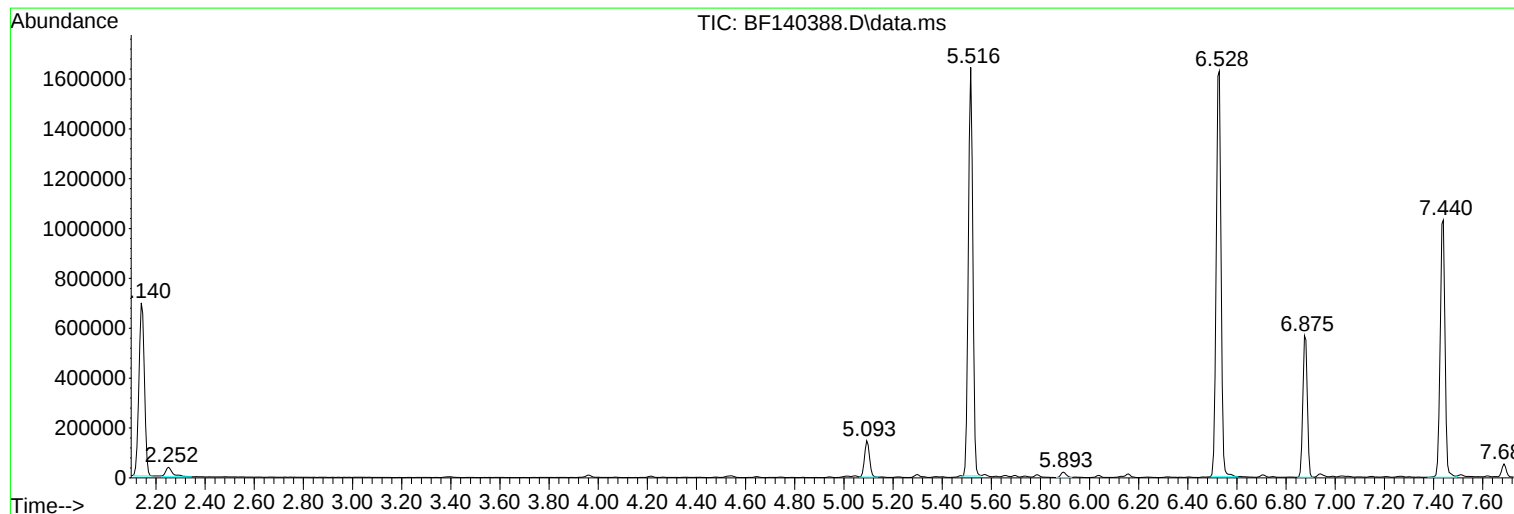
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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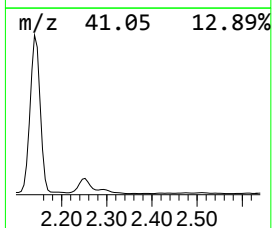
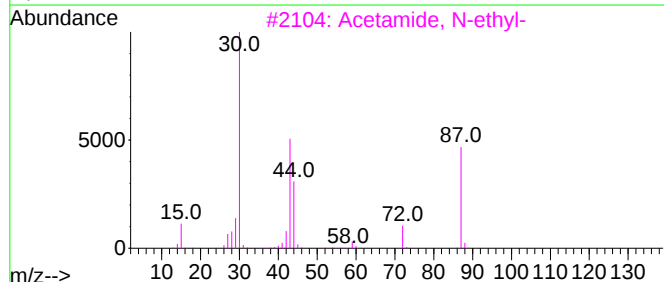
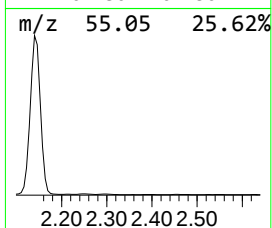
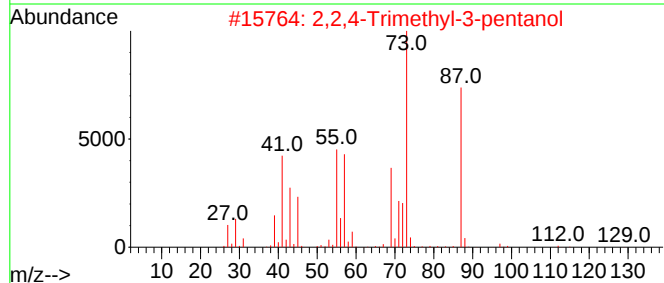
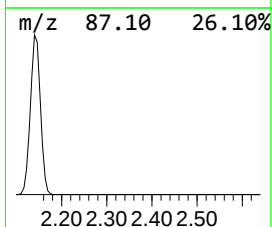
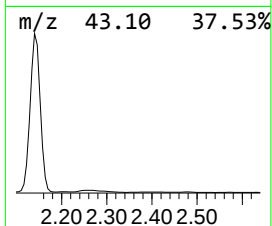
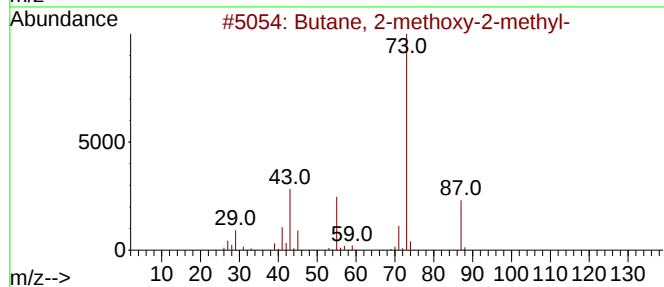
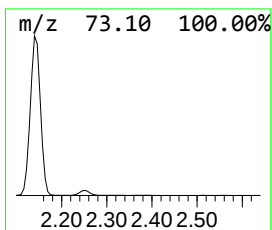
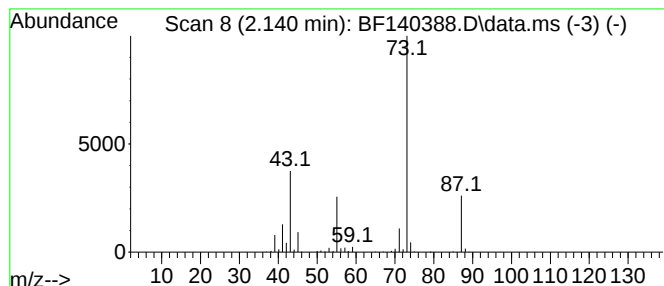
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.140	30.09 ng	1080310	1,4-Dichlorobenzene-d4	6.881

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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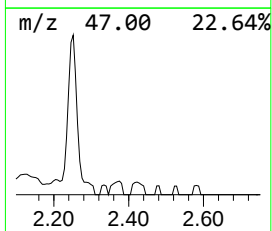
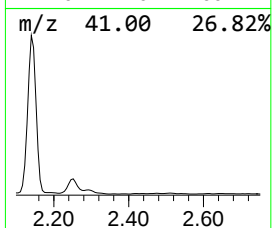
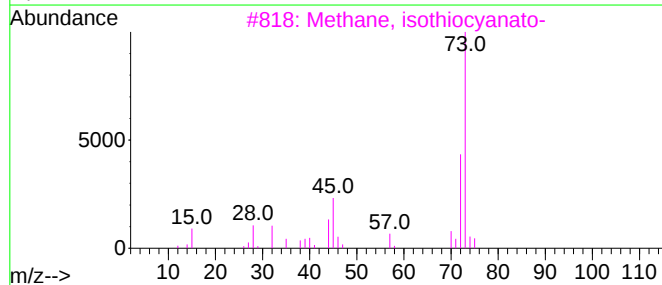
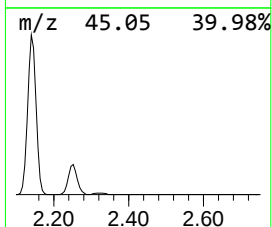
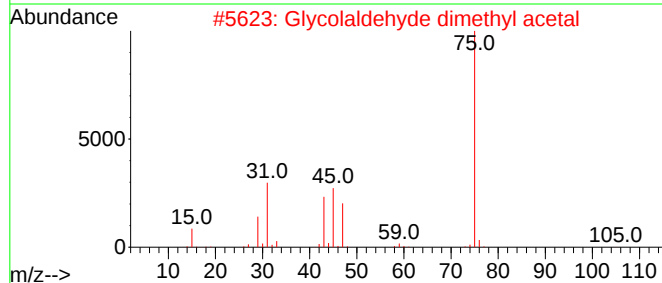
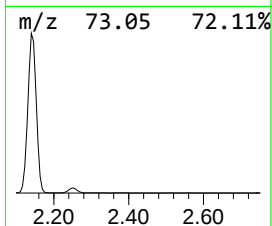
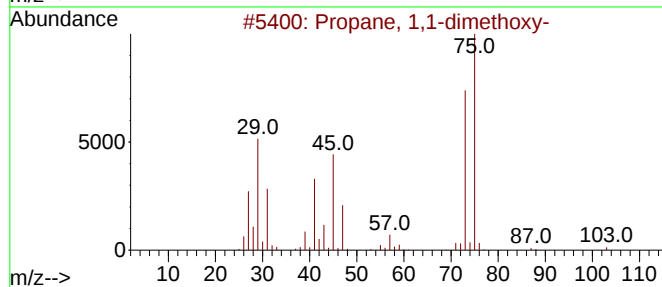
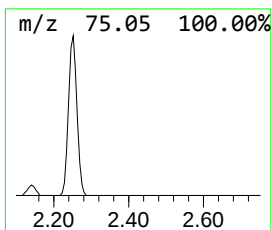
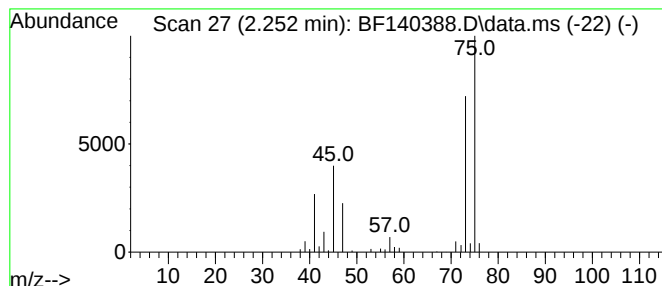
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.252	2.21 ng	79245	1,4-Dichlorobenzene-d4	6.881

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2			Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	56
3			Methane, isothiocyanato-	73	C2H3NS	000556-61-6	9
4			Glycine	75	C2H5NO2	000056-40-6	9
5			Methane, trimethoxy-	106	C4H10O3	000149-73-5	9



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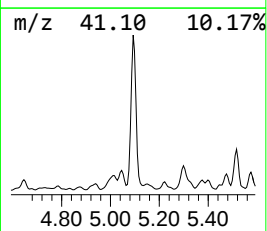
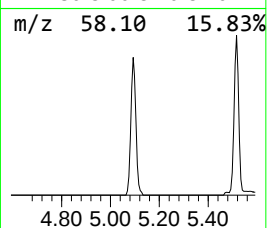
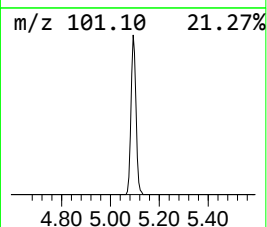
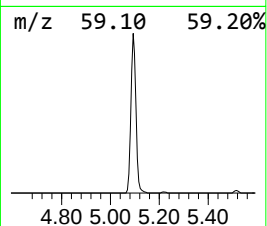
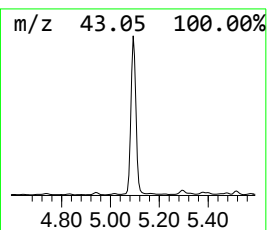
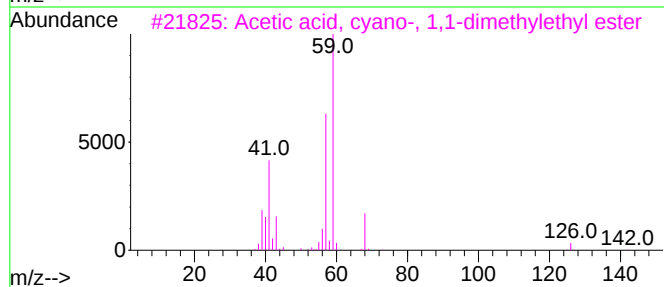
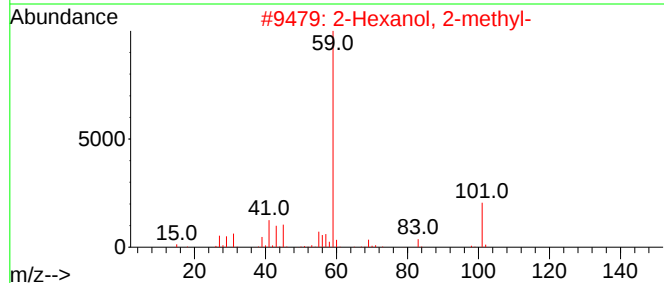
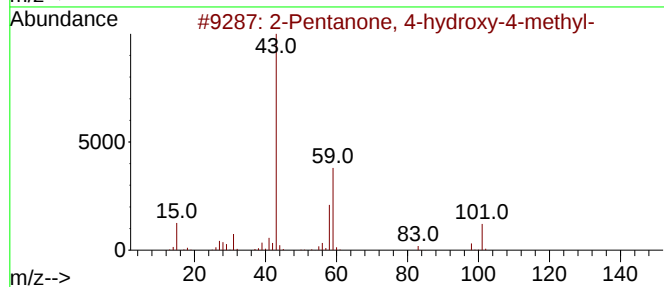
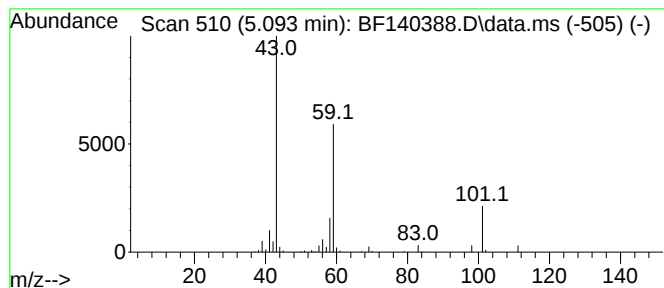
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	5.71 ng	205136	1,4-Dichlorobenzene-d4	6.881

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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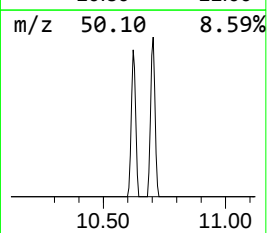
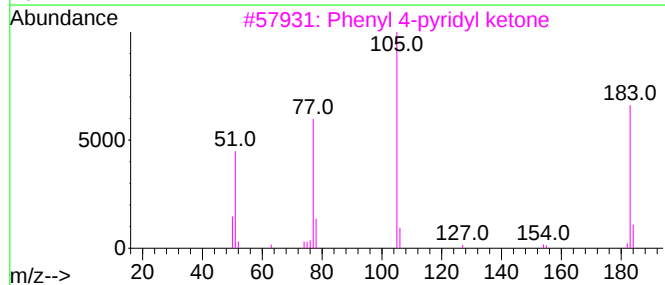
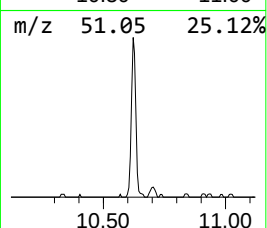
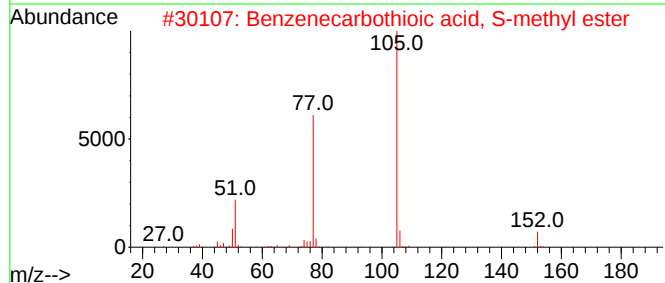
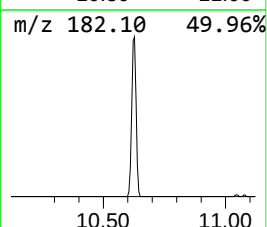
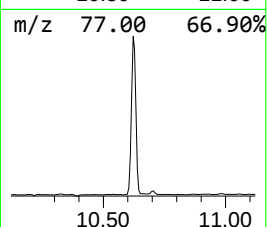
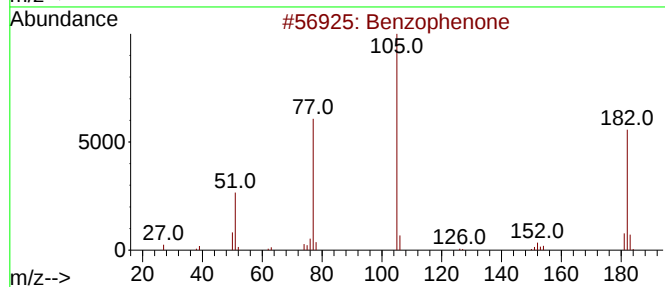
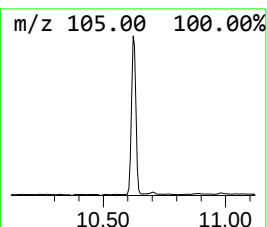
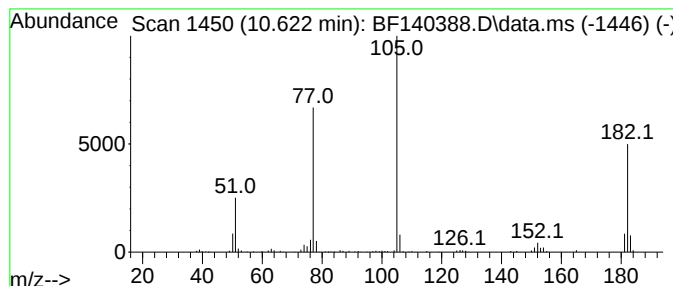
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.622	3.68 ng	148969	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	58
3			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	50
4			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	49
5			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49



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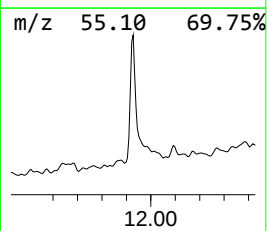
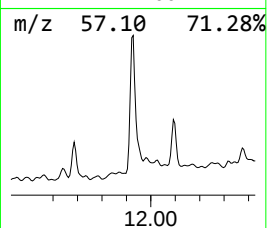
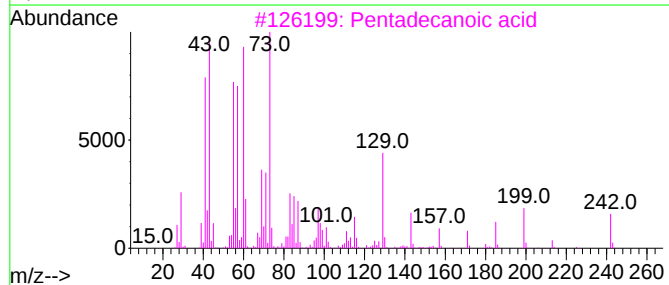
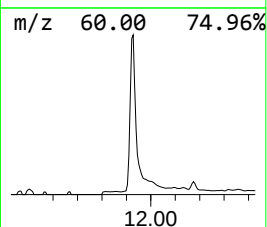
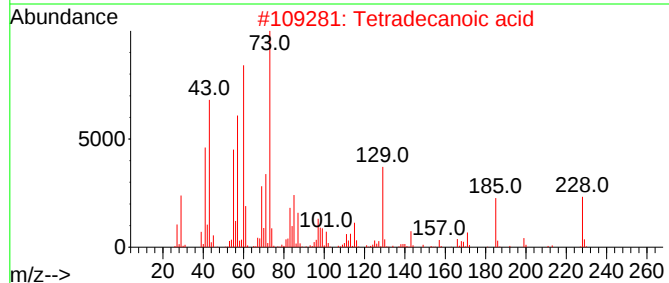
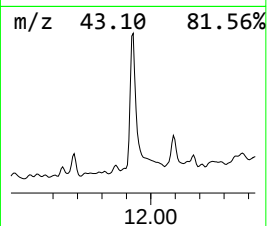
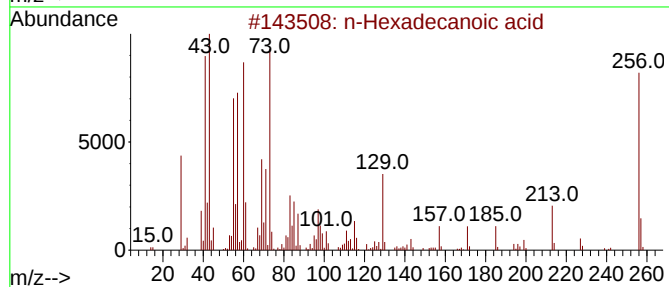
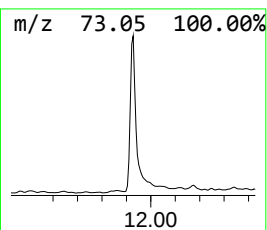
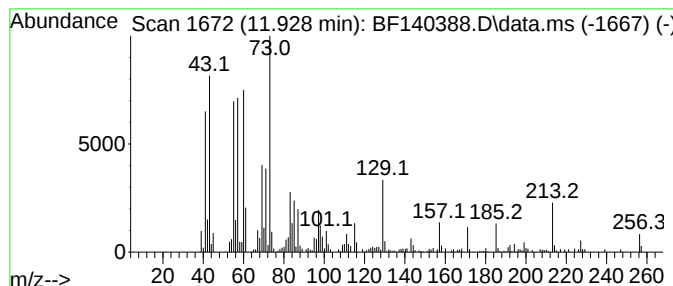
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.928	6.91 ng	264366	Phenanthrene-d10	11.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	83
5			Tridecanoic acid	214	C13H26O2	000638-53-9	83



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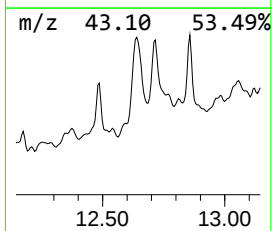
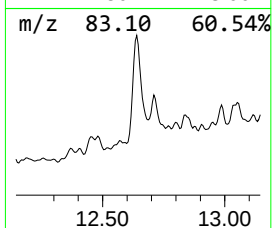
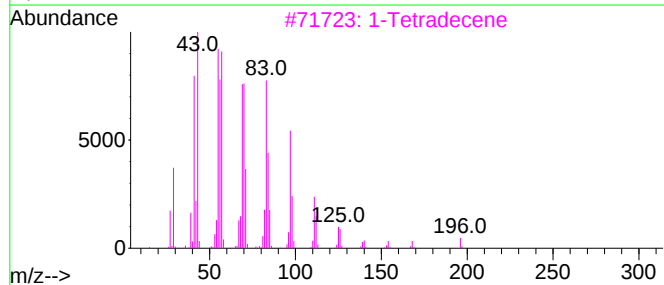
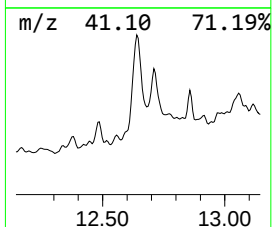
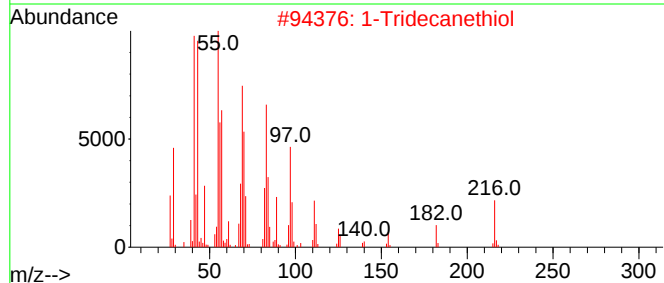
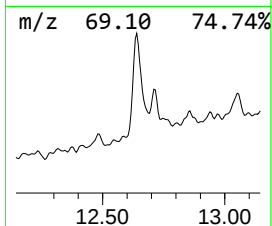
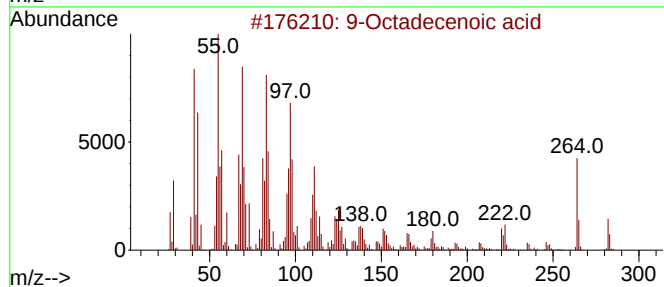
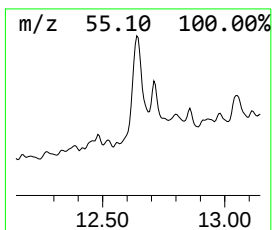
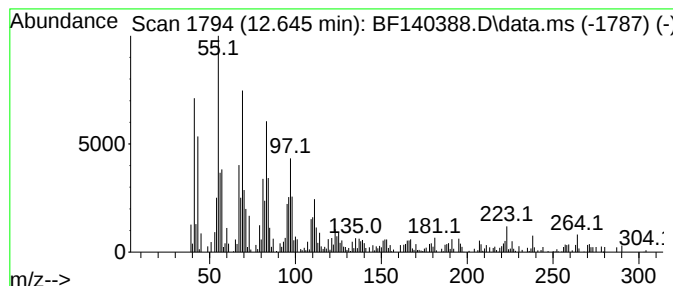
Instrument :
BNA_F
ClientSampleId :
BP-F21

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

Peak Number 6 9-Octadecenoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.645	7.35 ng	281521	Phenanthrene-d10	11.404	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid	282	C18H34O2	002027-47-6	91
2	1-Tridecanethiol	216	C13H28S	019484-26-5	86
3	1-Tetradecene	196	C14H28	001120-36-1	86
4	6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	86
5	1-Pentadecanethiol	244	C15H32S	025276-70-4	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111424\
Data File : BF140388.D
Acq On : 15 Nov 2024 02:42
Operator : RC/JU
Sample : P4789-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F21

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.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...	2.140	30.1	ng	1080310	1	6.881	718127	20.0
Propane, 1,1-di...	2.252	2.2	ng	79245	1	6.881	718127	20.0
2-Pentanone, 4-...	5.093	5.7	ng	205136	1	6.881	718127	20.0
Benzophenone	10.622	3.7	ng	148969	3	9.910	810176	20.0
n-Hexadecanoic ...	11.928	6.9	ng	264366	4	11.404	765574	20.0
9-Octadecenoic ...	12.645	7.3	ng	281521	4	11.404	765574	20.0