

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081425\
 Data File : BF143384.D
 Acq On : 14 Aug 2025 16:26
 Operator : RC/JU
 Sample : Q2814-06
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TW-82H-S

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-BF081225.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF143384.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.257	3	11	25	rVB	2497256	4002970	100.00%	16.942%
2	2.381	27	32	50	rVB2	20699	46481	1.16%	0.197%
3	5.157	497	504	516	rBV	217845	311677	7.79%	1.319%
4	5.563	568	573	586	rBV	1362247	1886147	47.12%	7.983%
5	6.563	737	743	770	rBV	1194400	1689290	42.20%	7.150%
6	6.769	770	778	790	rVV2	23263	43510	1.09%	0.184%
7	6.934	801	806	813	rBV	706828	880391	21.99%	3.726%
8	7.486	894	900	911	rBV	1220859	1630630	40.74%	6.901%
9	8.216	1018	1024	1039	rBV	940577	1294982	32.35%	5.481%
10	8.328	1039	1043	1050	rVV	231341	296165	7.40%	1.253%
11	8.433	1056	1061	1075	rVB2	45849	73688	1.84%	0.312%
12	8.798	1119	1123	1127	rBV2	33542	48638	1.22%	0.206%
13	9.286	1200	1206	1217	rBV	2053698	2574938	64.33%	10.898%
14	9.969	1316	1322	1333	rVB	1008644	1271399	31.76%	5.381%
15	10.339	1375	1385	1389	rBV	66356	105810	2.64%	0.448%
16	10.674	1437	1442	1451	rBV	464745	612876	15.31%	2.594%
17	10.757	1451	1456	1471	rBV	1114099	1481422	37.01%	6.270%
18	11.345	1552	1556	1561	rVB2	31093	41052	1.03%	0.174%
19	11.457	1570	1575	1582	rBV	857132	1121209	28.01%	4.745%
20	11.980	1659	1664	1679	rBV3	192499	358761	8.96%	1.518%
21	12.763	1792	1797	1806	rBV	44562	79965	2.00%	0.338%
22	12.933	1818	1826	1836	rVB3	23367	50847	1.27%	0.215%
23	13.039	1838	1844	1856	rVV	1344306	1743813	43.56%	7.380%
24	13.610	1937	1941	1949	rVB	40207	60413	1.51%	0.256%
25	13.939	1992	1997	2013	rBV	87501	181541	4.54%	0.768%
26	14.098	2019	2024	2035	rBV	488503	650633	16.25%	2.754%
27	14.251	2046	2050	2055	rBV	38856	54718	1.37%	0.232%
28	14.557	2098	2102	2120	rBV	40153	77247	1.93%	0.327%
29	14.868	2149	2155	2161	rBV2	34302	62502	1.56%	0.265%
30	15.221	2211	2215	2222	rBV	30586	44923	1.12%	0.190%
31	15.592	2272	2278	2288	rBV	480724	849090	21.21%	3.594%

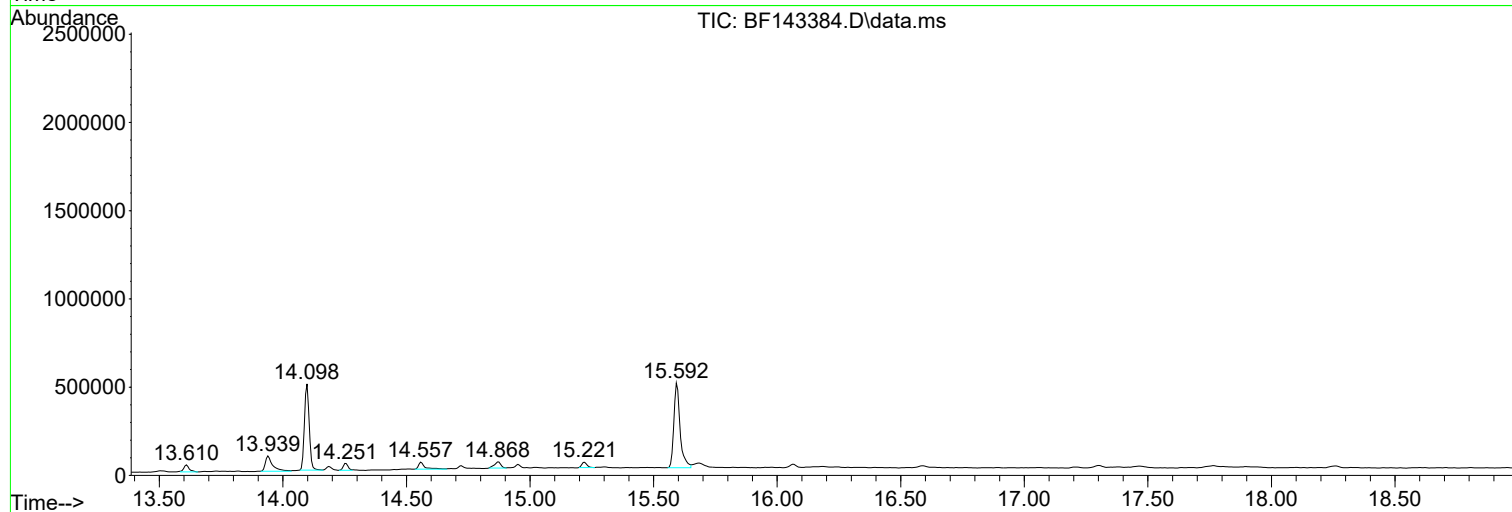
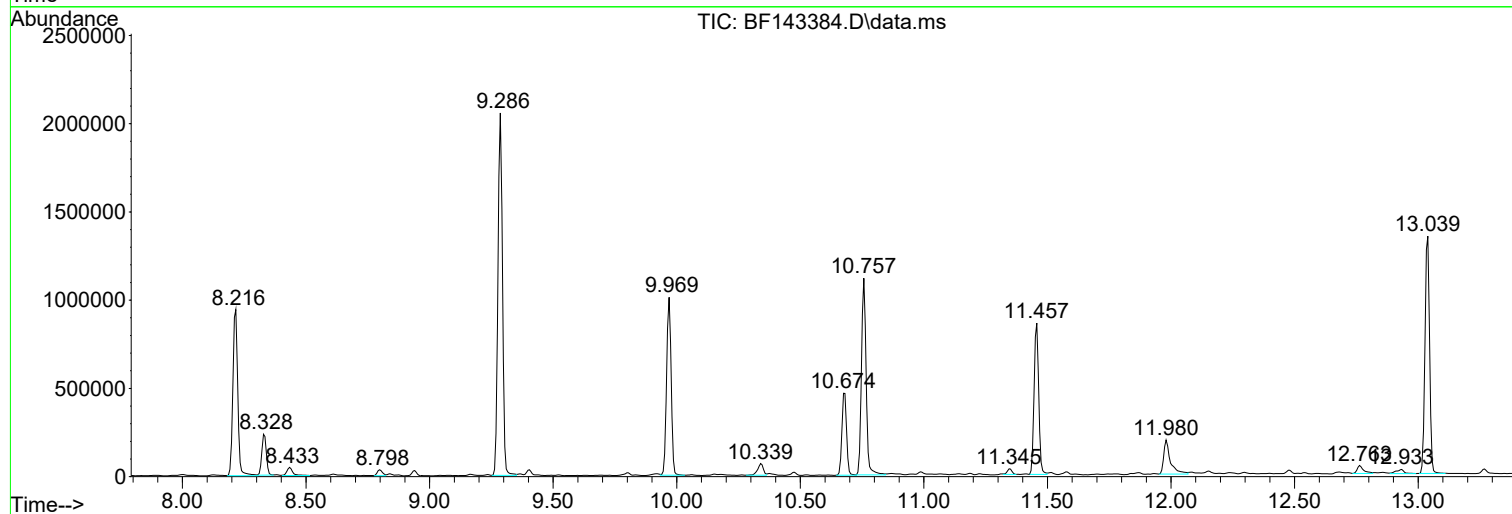
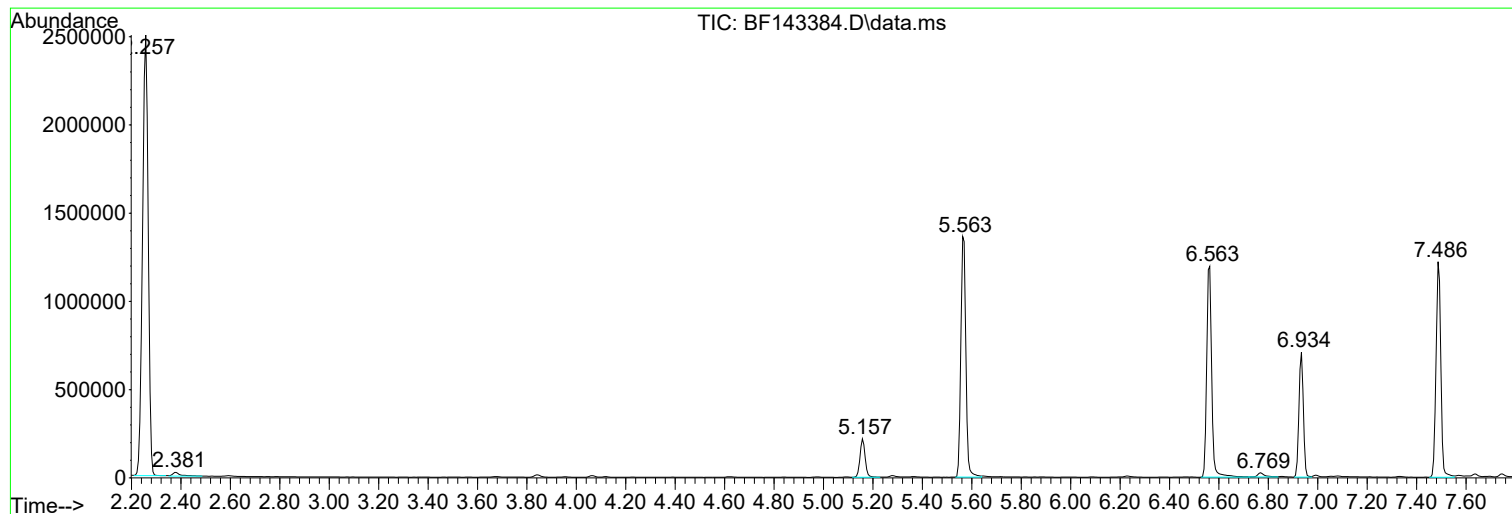
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081225.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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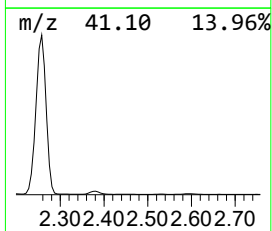
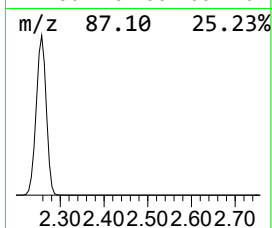
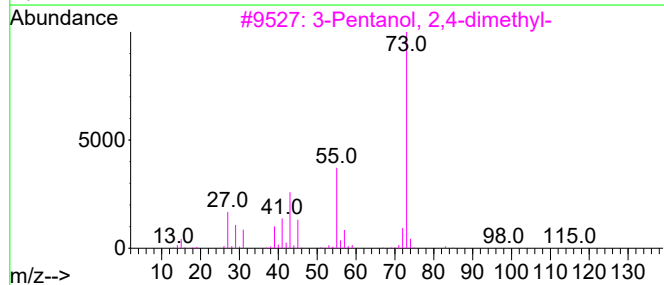
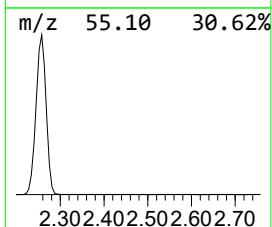
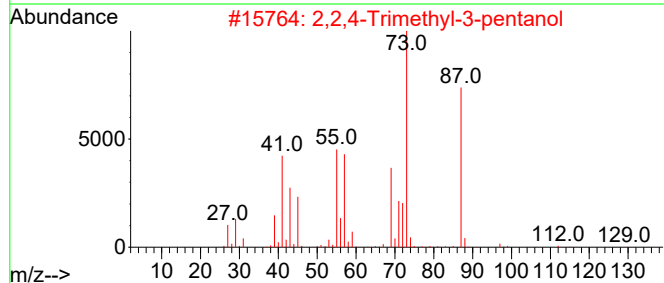
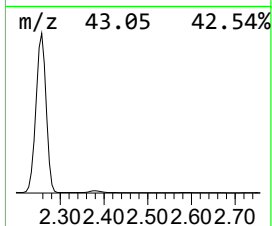
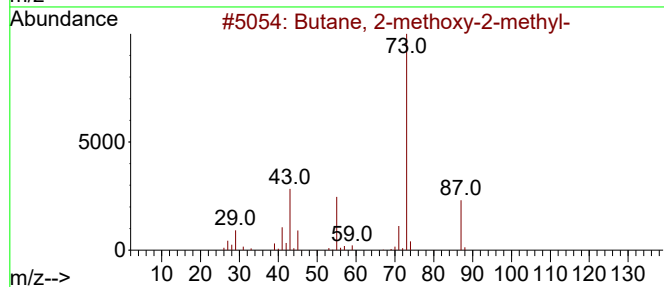
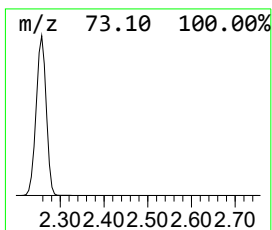
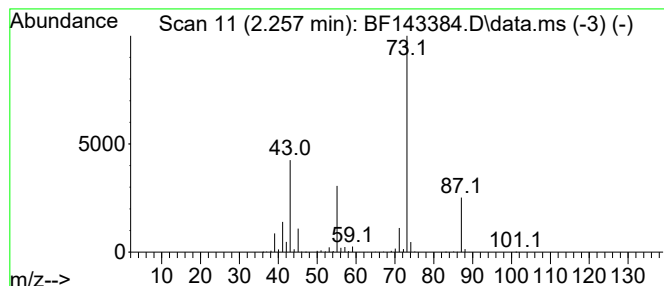
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.257	90.94 ng	4002970	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			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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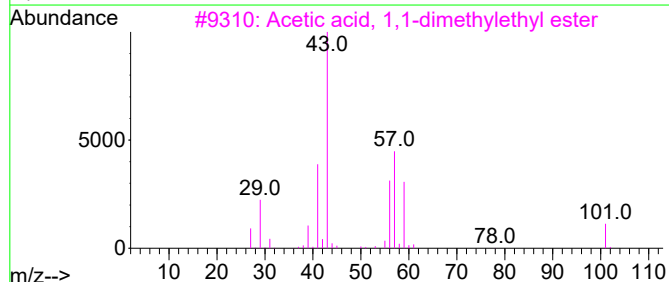
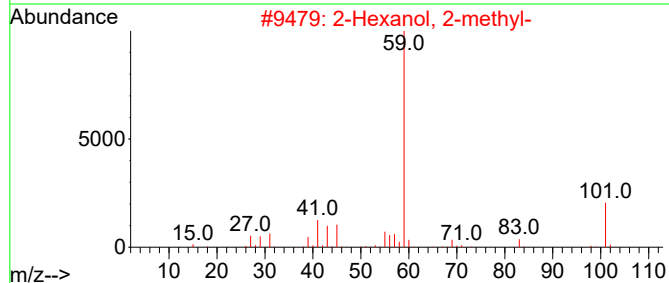
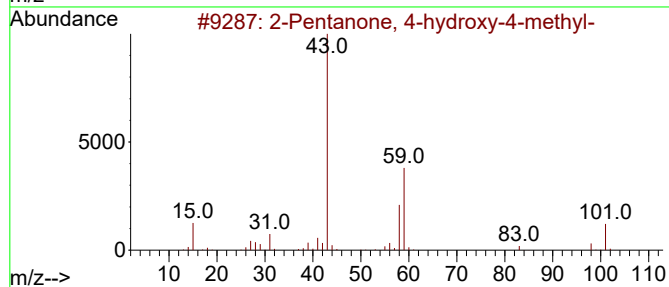
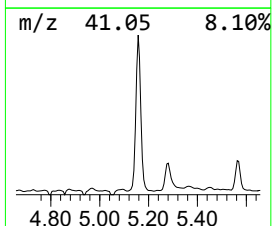
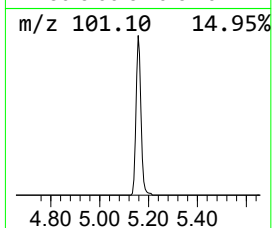
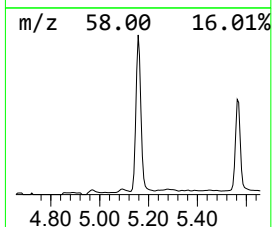
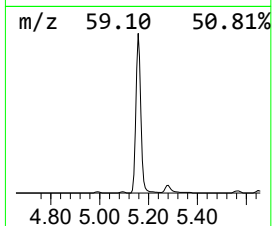
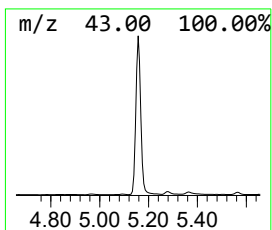
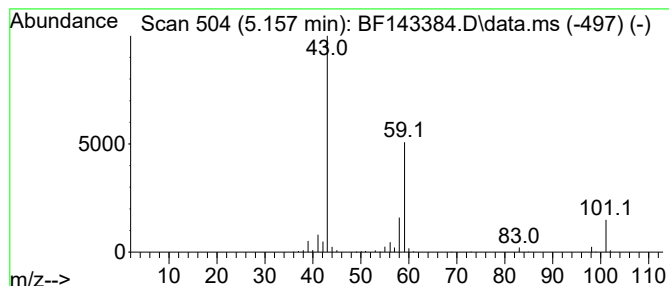
Instrument :
BNA_F
ClientSampleId :
TW-82H-S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081225.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 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.157	7.08 ng	311677	1,4-Dichlorobenzene-d4	6.934	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12



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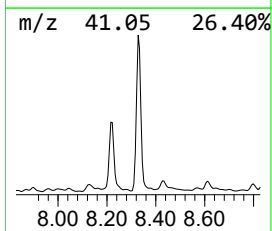
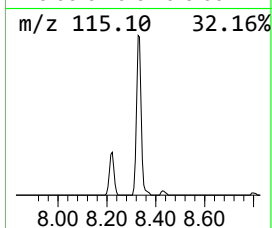
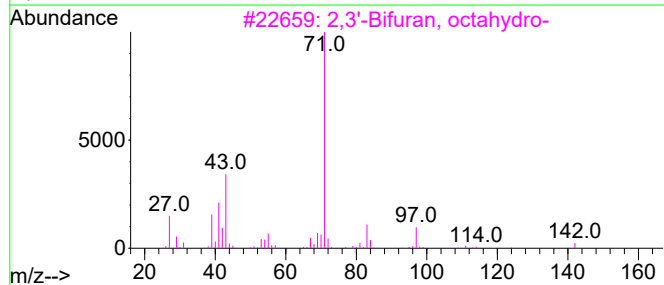
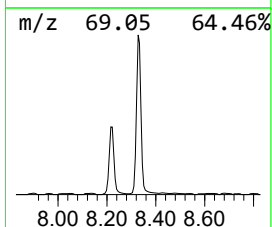
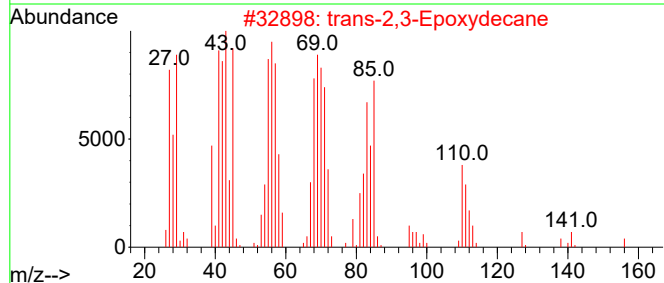
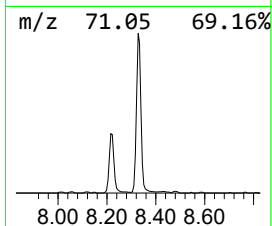
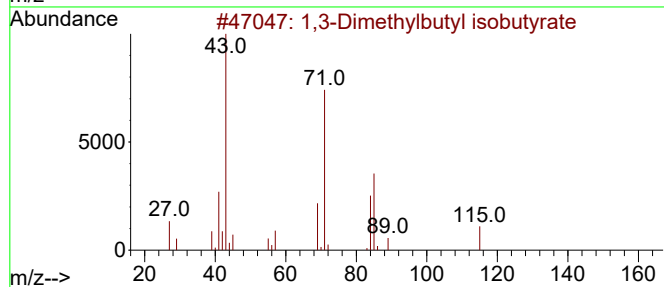
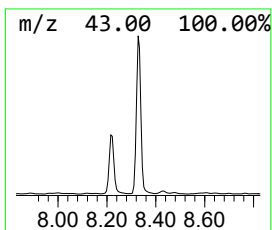
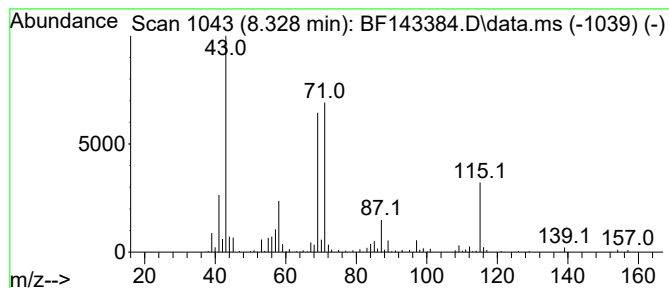
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown8.328 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.328	4.57 ng	296165	Naphthalene-d8	8.216

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dimethylbutyl isobutyrate	172	C10H20O2	1000429-31-6	43
2			trans-2,3-Epoxydecane	156	C10H20O	054125-39-2	38
3			2,3'-Bifuran, octahydro-	142	C8H14O2	073373-15-6	35
4			2-Ethoxytetrahydrofuran	116	C6H12O2	013436-46-9	35
5			1-Hydroxy-3-methyl-2-butanone	102	C5H10O2	036960-22-2	35



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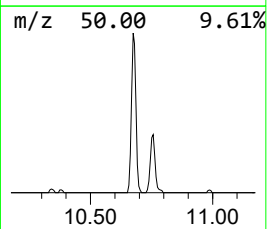
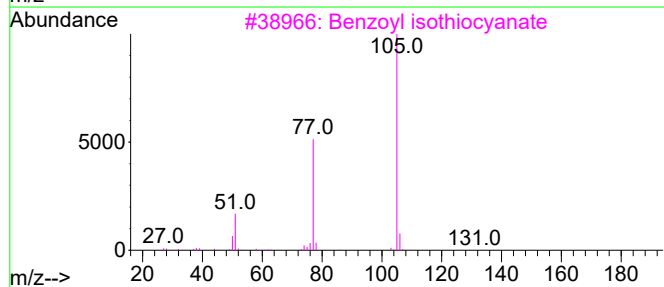
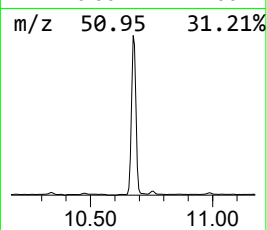
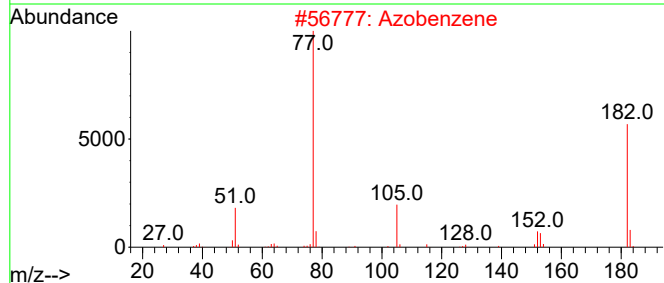
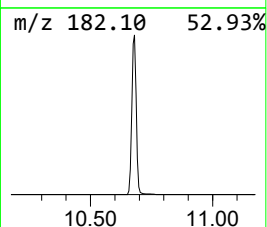
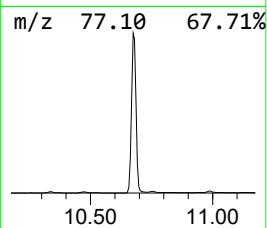
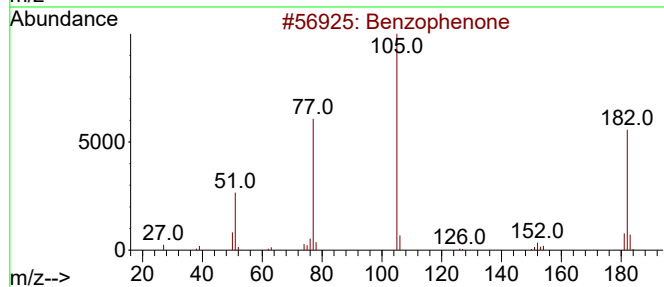
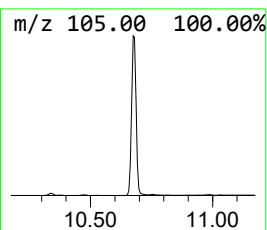
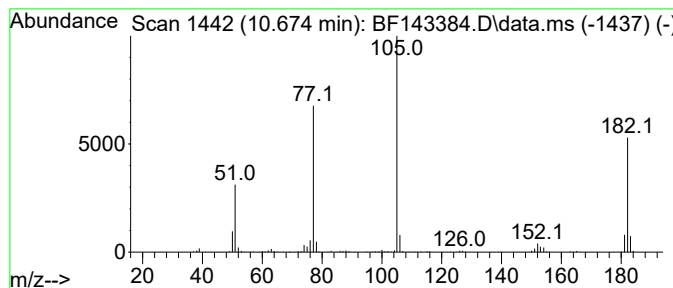
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.675	9.64 ng	612876	Acenaphthene-d10	9.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene	182	C12H10N2	000103-33-3	58
3			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	50
4			2-Phenyl-4-ethylidene-2-oxazolin...	187	C11H9NO2	037791-41-6	50
5			Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	50



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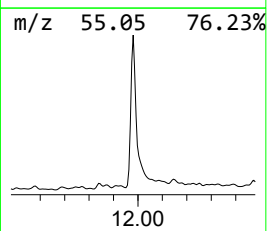
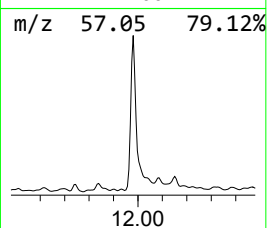
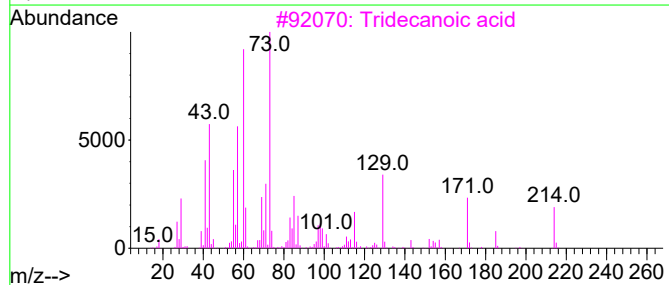
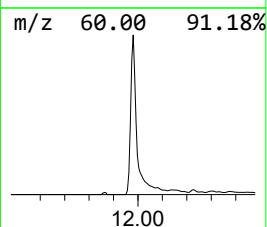
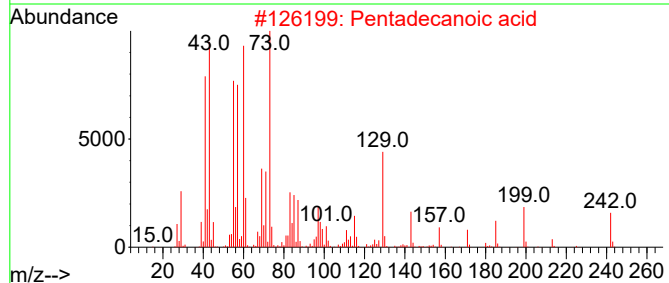
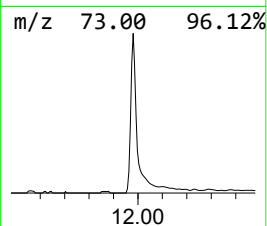
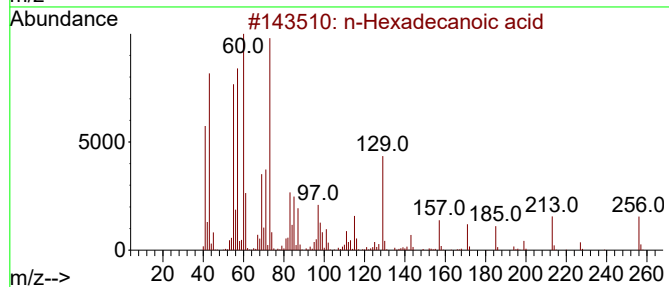
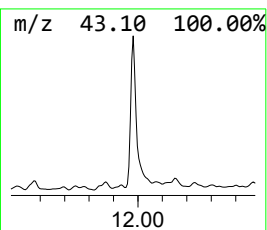
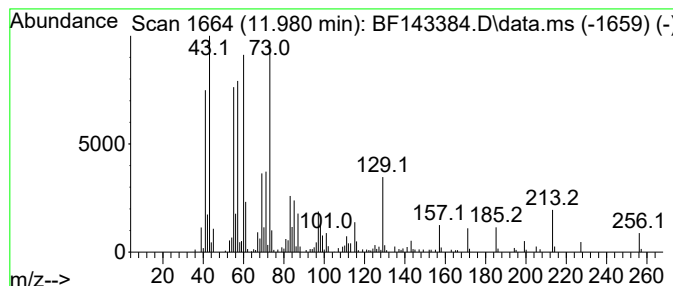
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.980	6.40 ng	358761	Phenanthrene-d10	11.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tridecanoic acid	214	C13H26O2	000638-53-9	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Undecanoic acid	186	C11H22O2	000112-37-8	58



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TW-82H-S

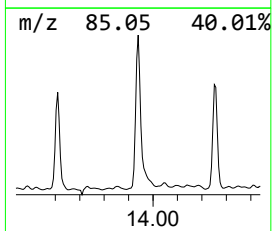
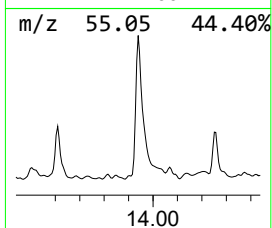
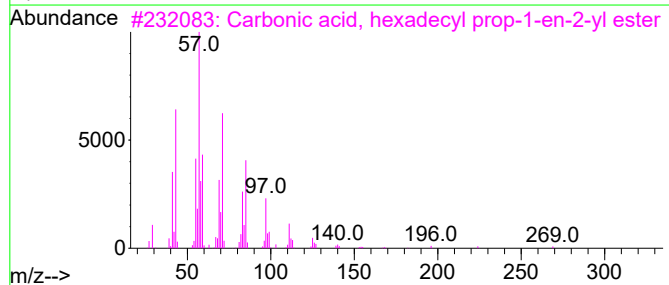
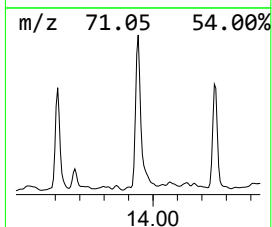
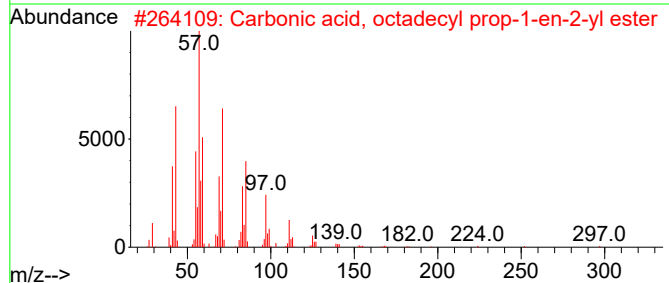
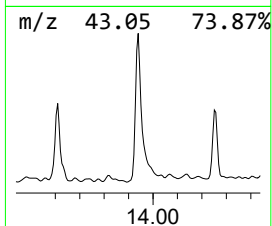
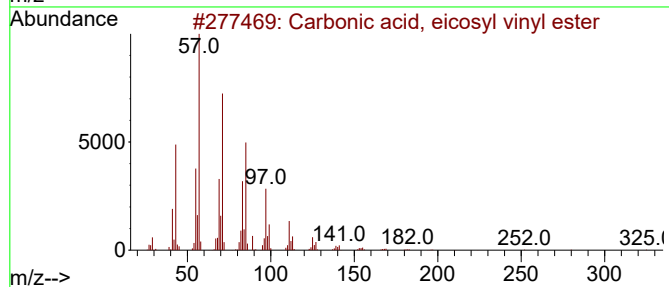
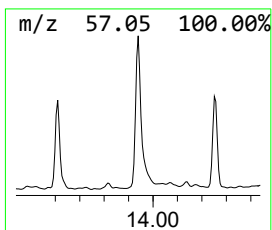
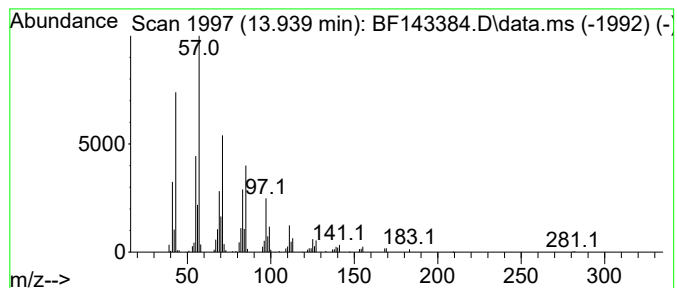
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Carbonic acid, eicosyl vinyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.939	5.58 ng	181541	Chrysene-d12	14.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	91
2			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	91
3			Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	91
4			Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	90
5			Carbonic acid, octadecyl vinyl e...	340	C21H40O3	1000382-54-4	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081425\
Data File : BF143384.D
Acq On : 14 Aug 2025 16:26
Operator : RC/JU
Sample : Q2814-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-82H-S

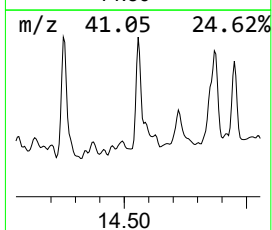
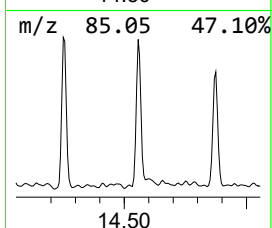
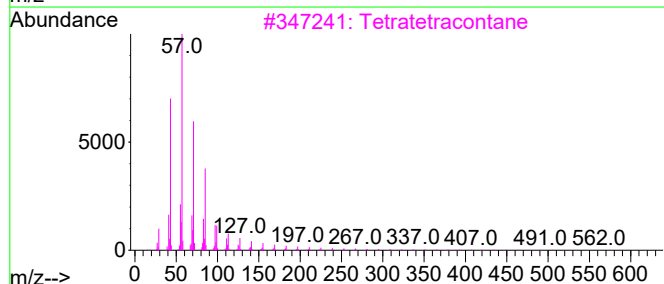
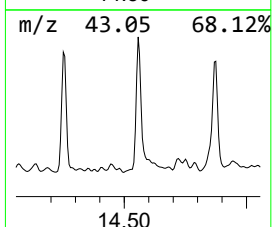
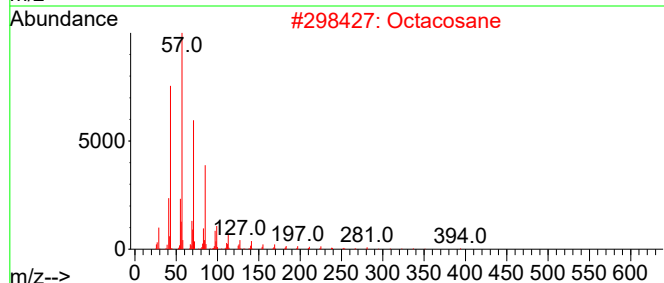
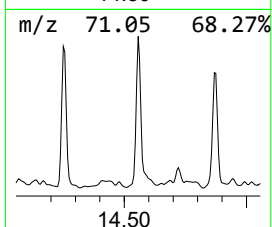
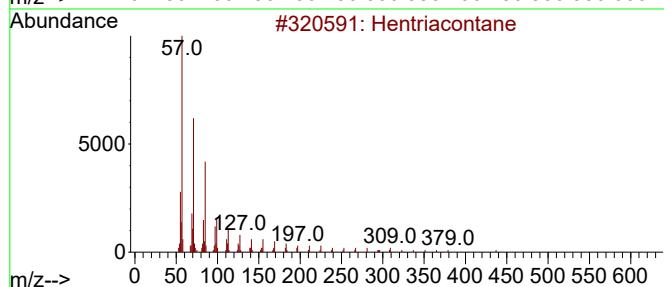
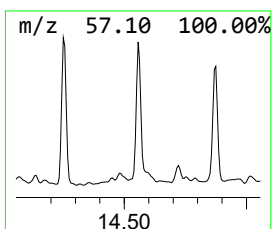
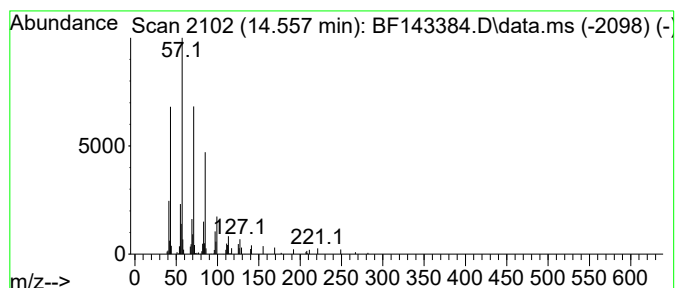
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hentriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.557	2.37 ng	77247	Chrysene-d12	14.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hentriacontane	437	C31H64	000630-04-6	91
2			Octacosane	394	C28H58	000630-02-4	91
3			Tetratetracontane	619	C44H90	007098-22-8	91
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5			Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081425\
Data File : BF143384.D
Acq On : 14 Aug 2025 16:26
Operator : RC/JU
Sample : Q2814-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-82H-S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081225.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...	2.257	90.9	ng	4002970	1	6.934	880391	20.0
2-Pentanone, 4-...	5.157	7.1	ng	311677	1	6.934	880391	20.0
unknown8.328	8.328	4.6	ng	296165	2	8.216	1294980	20.0
Benzophenone	10.675	9.6	ng	612876	3	9.969	1271400	20.0
n-Hexadecanoic ...	11.980	6.4	ng	358761	4	11.457	1121210	20.0
Carbonic acid, ...	13.939	5.6	ng	181541	5	14.098	650633	20.0
Hentriacontane	14.557	2.4	ng	77247	5	14.098	650633	20.0