

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091523\
 Data File : BF135280.D
 Acq On : 15 Sep 2023 15:40
 Operator : CG\JU
 Sample : 04409-16
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-6(0-6)COMP

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-BF091123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135280.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	6	18	rVB2	41244	61369	2.85%	0.381%
2	4.987	489	493	500	rVB	112523	143074	6.64%	0.888%
3	5.393	557	562	565	rBV	2113597	1978103	91.74%	12.277%
4	6.398	729	733	736	rBV	2018153	1971302	91.42%	12.234%
5	6.593	763	766	772	rBV	39694	44559	2.07%	0.277%
6	6.757	790	794	798	rBV	776829	602397	27.94%	3.739%
7	7.293	881	885	886	rBV	44247	34123	1.58%	0.212%
8	7.322	886	890	893	rVB	1372557	1232424	57.15%	7.649%
9	8.034	1007	1011	1015	rBV	909346	788014	36.54%	4.891%
10	9.116	1190	1195	1198	rBV	2469203	2156285	100.00%	13.382%
11	9.234	1211	1215	1218	rBV	41555	36686	1.70%	0.228%
12	9.792	1306	1310	1314	rBV	1033859	848637	39.36%	5.267%
13	10.586	1441	1445	1448	rBV	1433478	1233439	57.20%	7.655%
14	11.286	1560	1564	1567	rBV	994089	846443	39.25%	5.253%
15	11.822	1650	1655	1667	rBV	301592	332977	15.44%	2.067%
16	12.504	1769	1771	1782	rBV6	8877	26231	1.22%	0.163%
17	12.610	1786	1789	1798	rBV	89247	110580	5.13%	0.686%
18	12.880	1831	1835	1839	rBV	1911818	1776206	82.37%	11.024%
19	13.804	1987	1992	2004	rBV2	105604	238461	11.06%	1.480%
20	13.939	2012	2015	2019	rBV	622845	578184	26.81%	3.588%
21	14.116	2041	2045	2048	rBV	25746	27212	1.26%	0.169%
22	14.421	2093	2097	2099	rBV	49644	50440	2.34%	0.313%
23	14.457	2099	2103	2111	rVB2	34977	69894	3.24%	0.434%
24	14.727	2146	2149	2153	rVB	49827	43109	2.00%	0.268%
25	14.798	2158	2161	2167	rVB6	16484	24662	1.14%	0.153%
26	15.063	2202	2206	2211	rBV	55260	64238	2.98%	0.399%
27	15.410	2260	2265	2269	rBV	555717	668247	30.99%	4.147%
28	15.445	2269	2271	2276	rVB3	37987	43963	2.04%	0.273%
29	15.886	2341	2346	2350	rVB	37306	55945	2.59%	0.347%
30	16.398	2429	2433	2436	rBV5	16093	25538	1.18%	0.158%

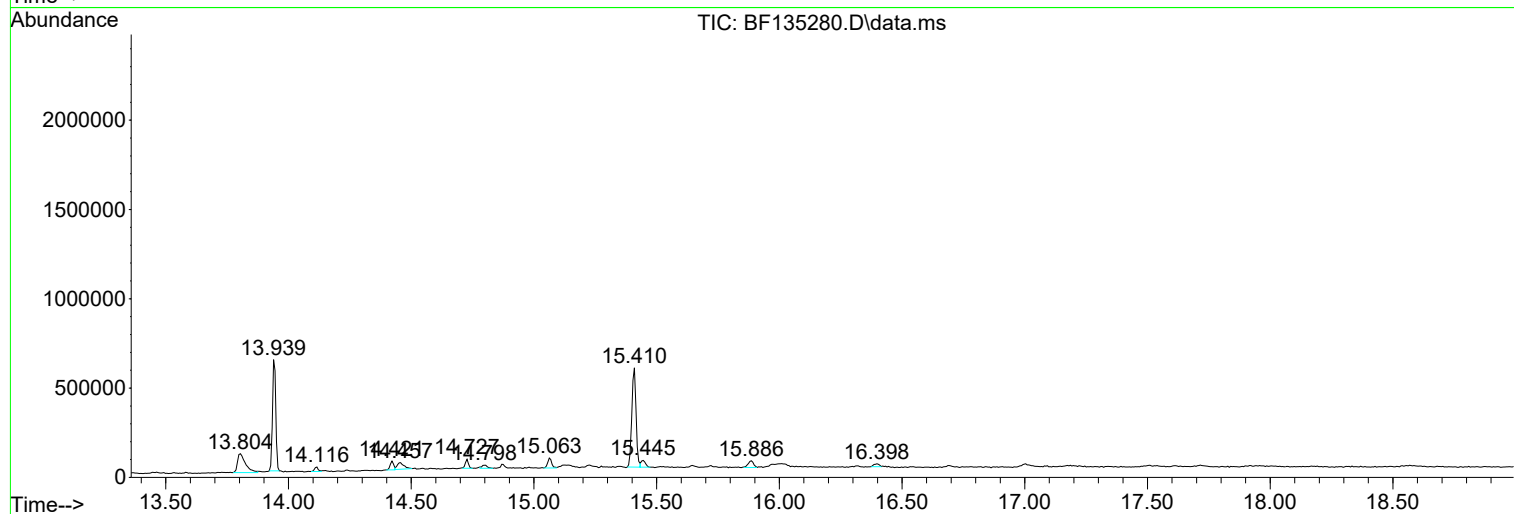
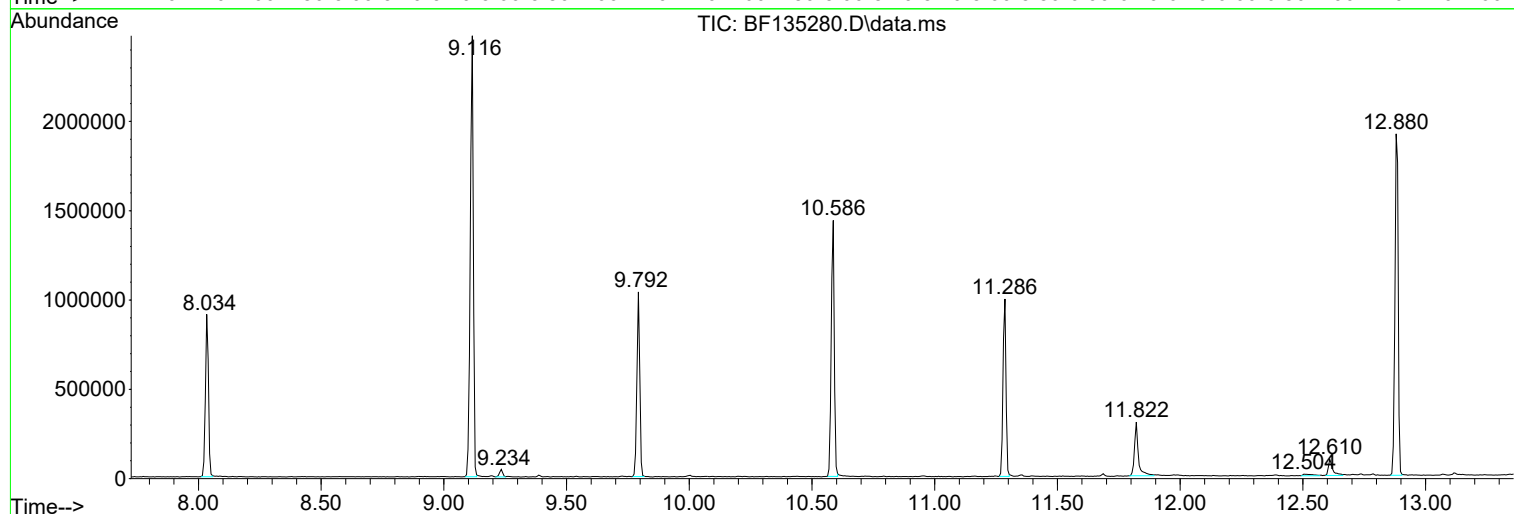
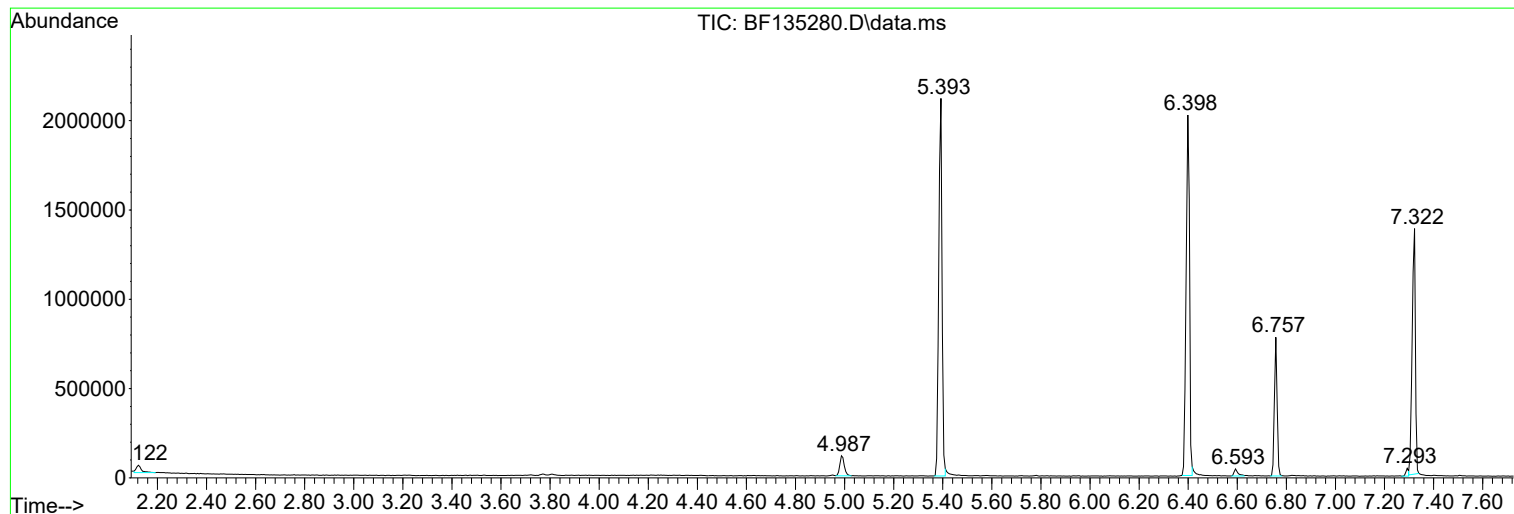
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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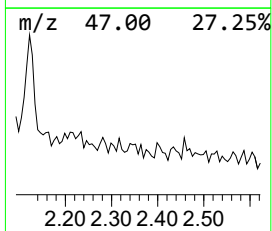
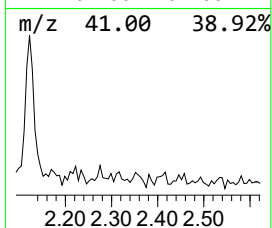
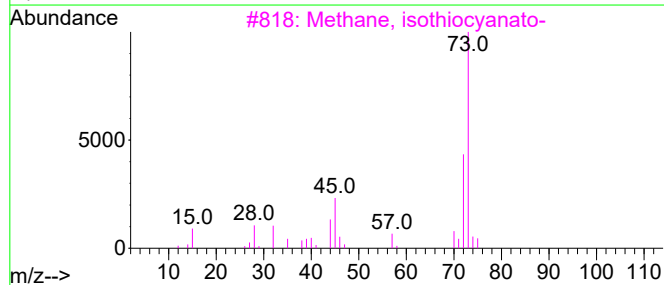
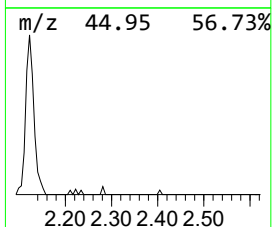
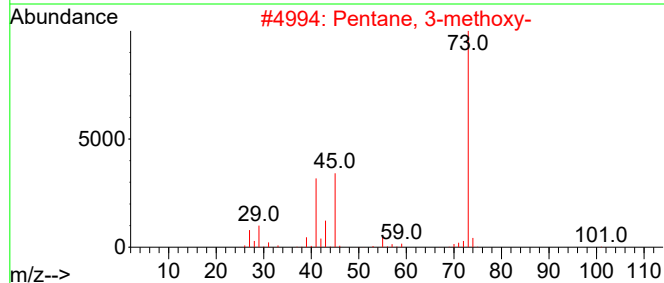
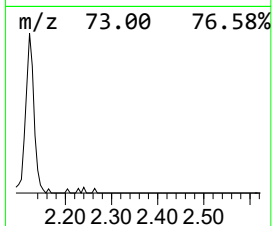
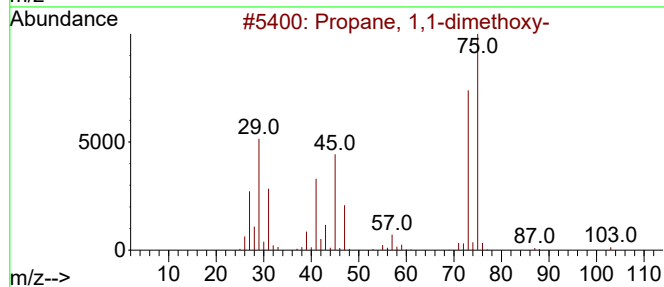
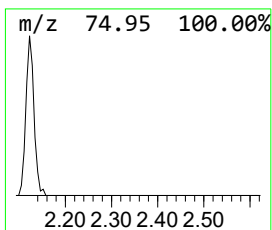
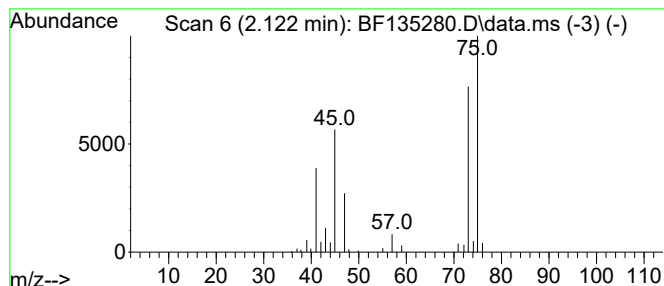
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.122	2.04 ng	61369	1,4-Dichlorobenzene-d4	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	27
3			Methane, isothiocyanato-	73	C2H3NS	000556-61-6	9
4			1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	9
5			Silanol, trimethyl-	90	C3H10OSi	001066-40-6	9



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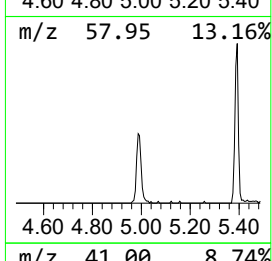
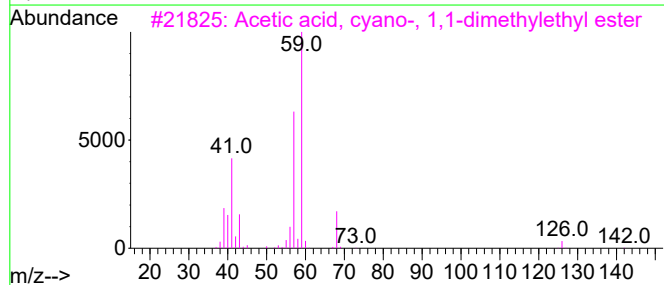
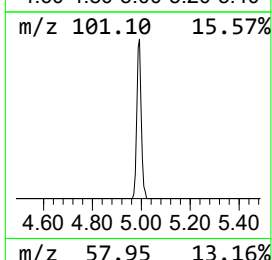
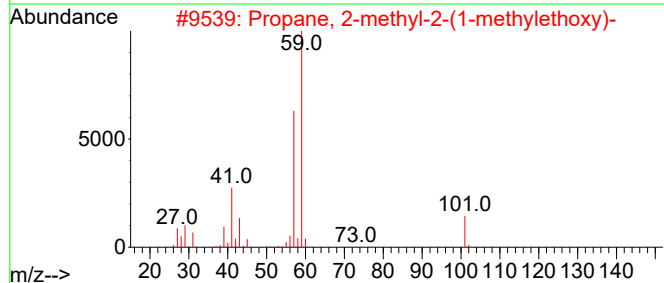
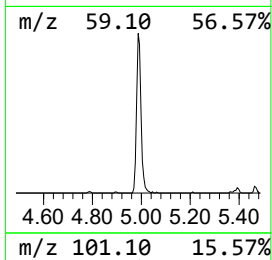
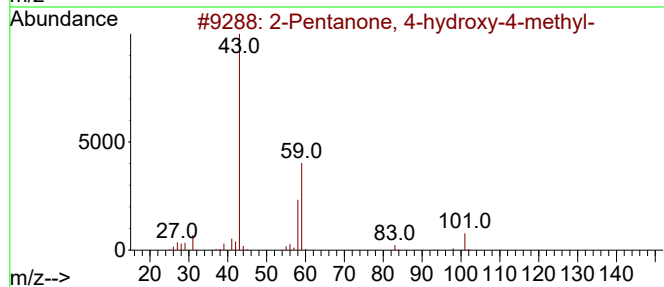
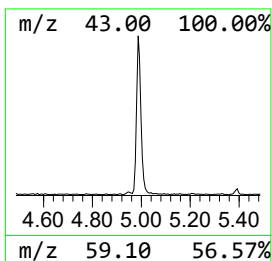
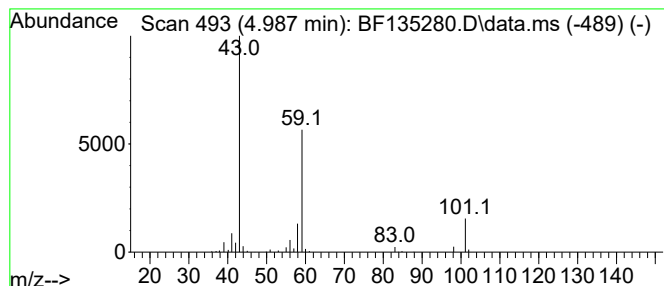
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.987	4.75 ng	143074	1,4-Dichlorobenzene-d4	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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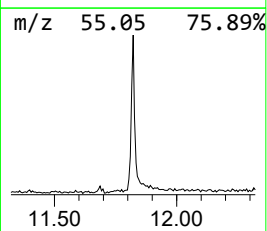
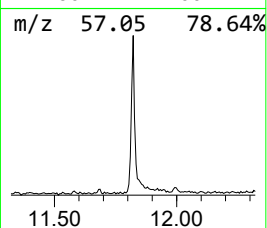
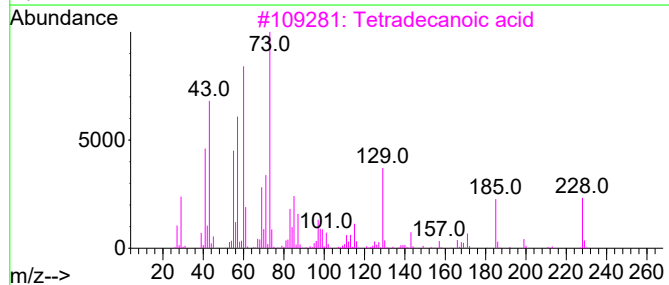
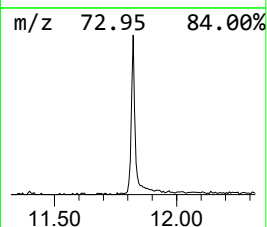
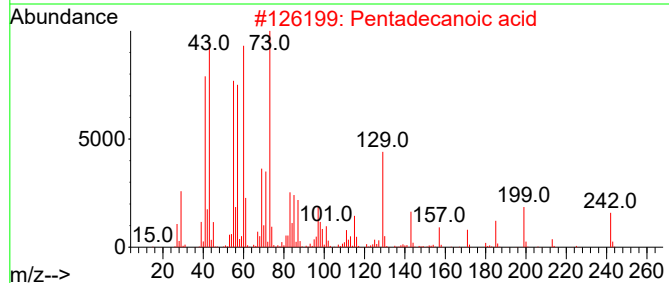
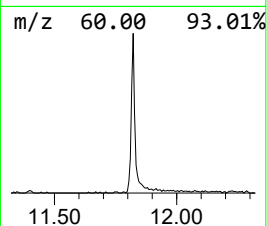
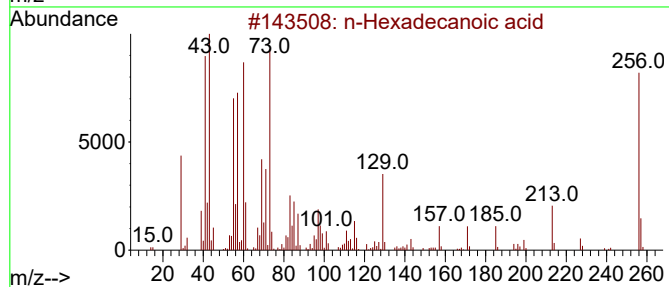
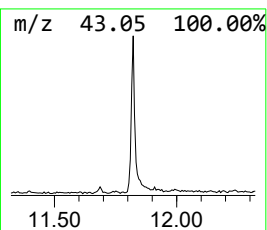
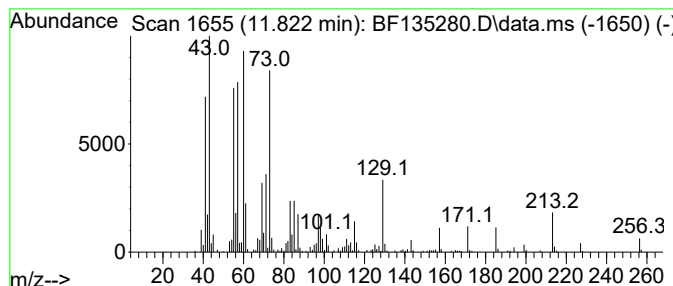
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.822	7.87 ng	332977	Phenanthrene-d10	11.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4			Tridecanoic acid	214	C13H26O2	000638-53-9	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	50



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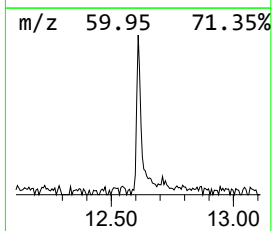
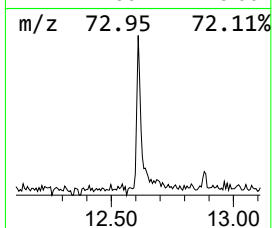
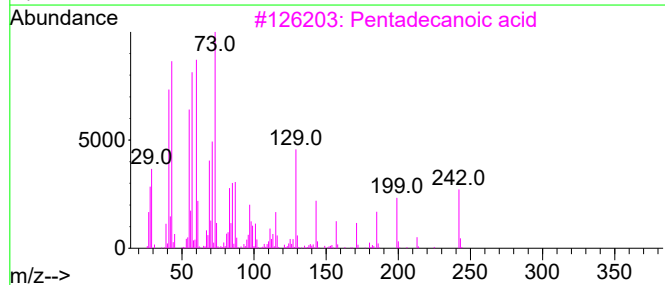
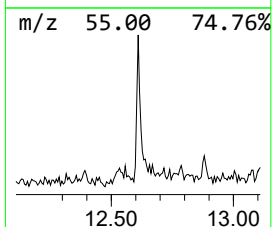
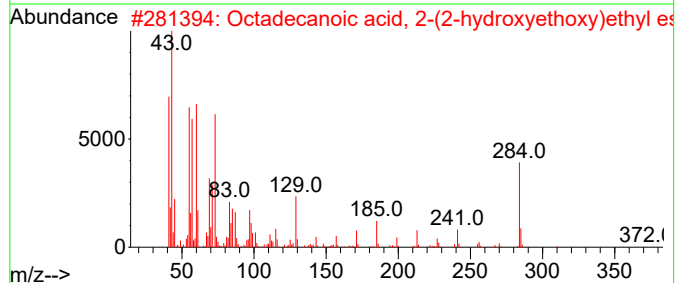
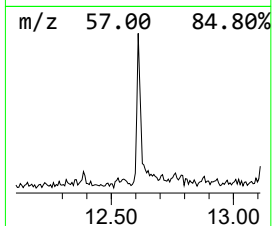
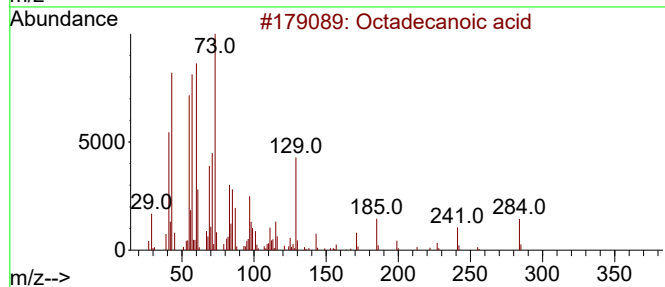
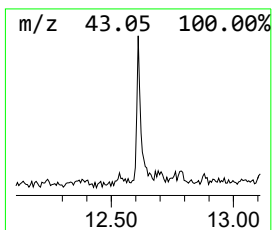
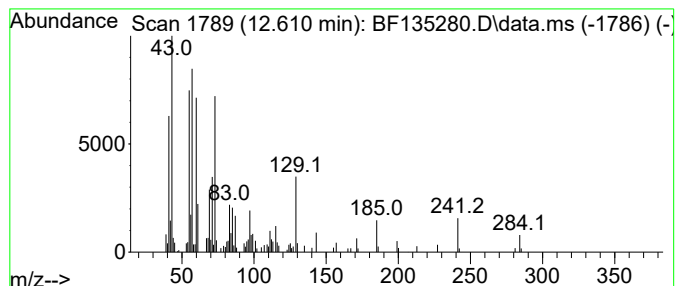
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Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.610	2.61 ng	110580	Phenanthrene-d10	11.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	58



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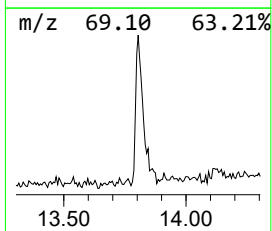
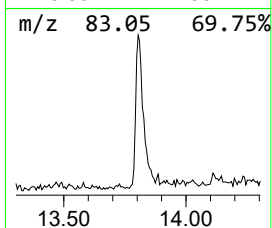
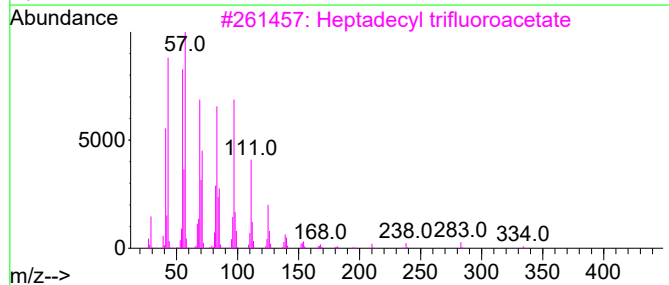
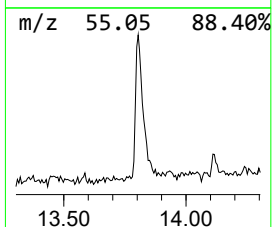
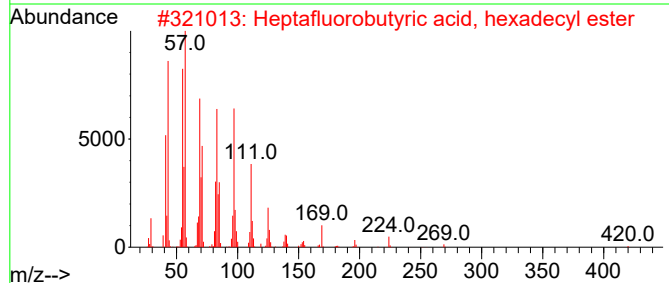
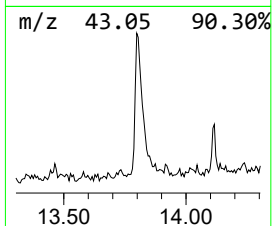
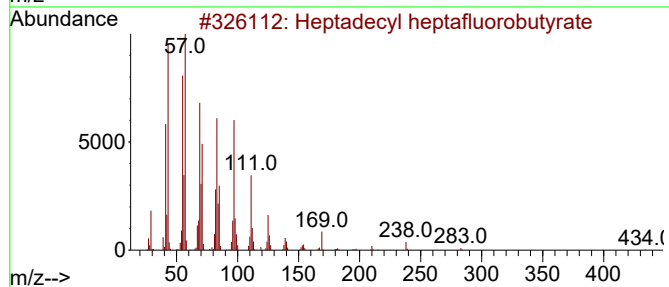
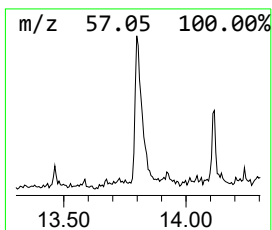
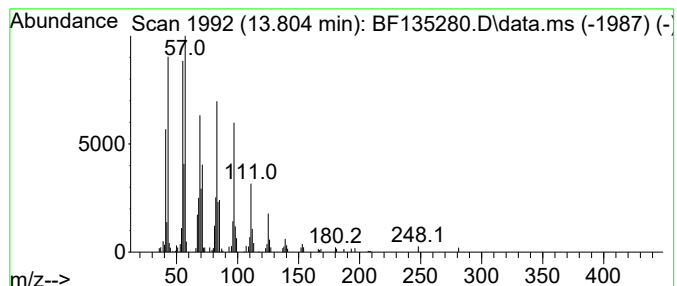
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Heptadecyl heptafluorobutyrate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.804	8.25 ng	238461	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	95
2			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
3			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
4			1-Heneicosanol	312	C21H44O	015594-90-8	93
5			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91



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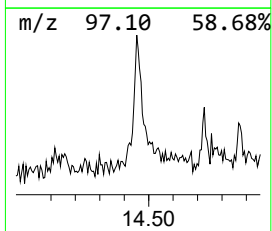
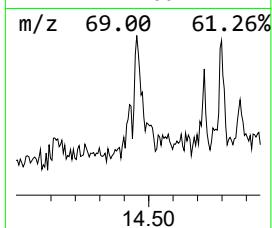
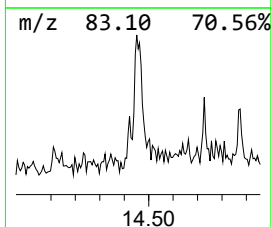
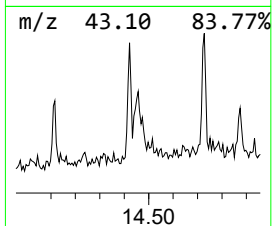
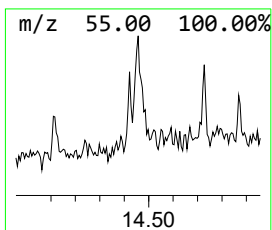
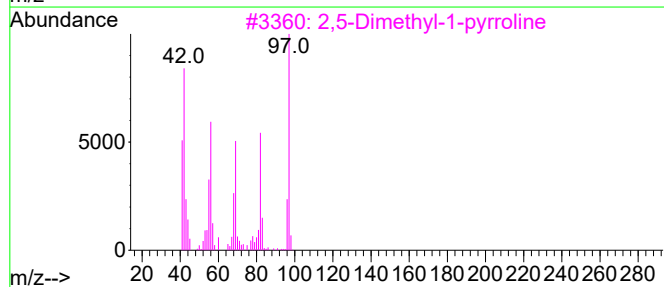
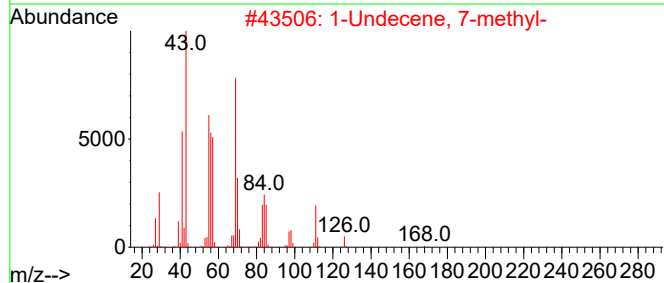
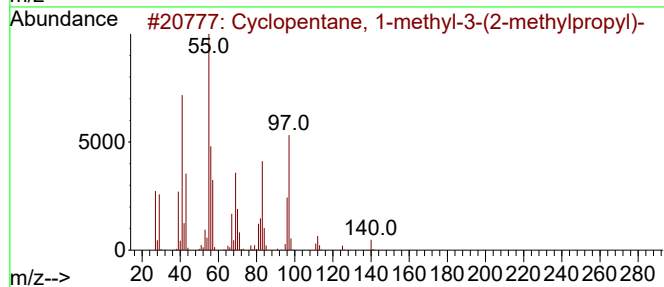
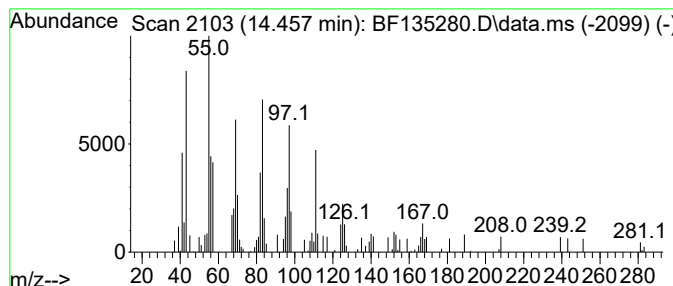
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown14.457 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.457	2.42 ng	69894	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1-methyl-3-(2-meth...	140	C10H20	029053-04-1	43
2			1-Undecene, 7-methyl-	168	C12H24	074630-42-5	41
3			2,5-Dimethyl-1-pyrroline	97	C6H11N	000822-64-0	38
4			Cyclohexane, 1,1,2-trimethyl-	126	C9H18	007094-26-0	30
5			Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091523\
Data File : BF135280.D
Acq On : 15 Sep 2023 15:40
Operator : CG\JU
Sample : 04409-16
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-6(0-6)COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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
Propane, 1,1-di...	2.122	2.0	ng	61369	1	6.757	602397	20.0
2-Pentanone, 4-...	4.987	4.8	ng	143074	1	6.757	602397	20.0
n-Hexadecanoic ...	11.822	7.9	ng	332977	4	11.286	846443	20.0
Octadecanoic acid	12.610	2.6	ng	110580	4	11.286	846443	20.0
Heptadecyl hept...	13.804	8.3	ng	238461	5	13.939	578184	20.0
unknown14.457	14.457	2.4	ng	69894	5	13.939	578184	20.0