

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100523\
 Data File : BF135610.D
 Acq On : 05 Oct 2023 20:47
 Operator : CG\JU
 Sample : 04714-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-1

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: BF135610.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.769	282	286	298	rVB	17874	30878	1.10%	0.143%
2	4.963	484	489	506	rBV	923334	1206122	42.87%	5.571%
3	5.375	556	559	584	rBV	2818835	2813505	100.00%	12.994%
4	5.757	620	624	630	rBV	29845	35679	1.27%	0.165%
5	6.387	728	731	755	rBV	2551666	2715355	96.51%	12.541%
6	6.581	759	764	778	rBV	43736	84982	3.02%	0.392%
7	6.740	787	791	801	rBV	954355	820392	29.16%	3.789%
8	7.304	883	887	890	rBV	1969857	1654627	58.81%	7.642%
9	8.016	1005	1008	1023	rVB	1273703	1046312	37.19%	4.832%
10	9.092	1187	1191	1194	rBV	2900552	2458388	87.38%	11.354%
11	9.216	1207	1212	1220	rBV	654969	666009	23.67%	3.076%
12	9.769	1303	1306	1310	rBV	1097823	945813	33.62%	4.368%
13	10.569	1438	1442	1451	rBV	1244361	1242709	44.17%	5.739%
14	11.263	1557	1560	1563	rBV	862378	769654	27.36%	3.555%
15	11.286	1563	1564	1568	rVB	58757	50021	1.78%	0.231%
16	11.804	1649	1652	1663	rBV2	243208	321517	11.43%	1.485%
17	12.486	1765	1768	1771	rBV	149281	125066	4.45%	0.578%
18	12.592	1783	1786	1792	rBV2	49172	74409	2.64%	0.344%
19	12.716	1802	1807	1812	rVB	123122	134080	4.77%	0.619%
20	12.857	1827	1831	1835	rBV	1697741	1568013	55.73%	7.242%
21	13.433	1925	1929	1932	rBV2	30538	33636	1.20%	0.155%
22	13.769	1983	1986	1987	rBV2	35146	31958	1.14%	0.148%
23	13.804	1987	1992	2006	rVV8	69776	272249	9.68%	1.257%
24	13.927	2008	2013	2016	rVV	803228	839099	29.82%	3.875%
25	13.951	2016	2017	2022	rVB	90834	64462	2.29%	0.298%
26	14.086	2037	2040	2043	rBV2	32951	31259	1.11%	0.144%
27	14.392	2089	2092	2095	rVB	56892	54239	1.93%	0.251%
28	14.451	2097	2102	2106	rBV3	84183	143415	5.10%	0.662%
29	14.698	2141	2144	2147	rVB	36857	39393	1.40%	0.182%
30	14.968	2186	2190	2193	rBV	88961	123719	4.40%	0.571%
31	15.027	2197	2200	2204	rVB	158539	179615	6.38%	0.830%
32	15.268	2238	2241	2246	rVB	49804	57844	2.06%	0.267%
33	15.333	2248	2252	2257	rVB	61676	69798	2.48%	0.322%
34	15.392	2257	2262	2273	rBV	574723	788165	28.01%	3.640%
35	15.839	2333	2338	2344	rVB	104305	159563	5.67%	0.737%

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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

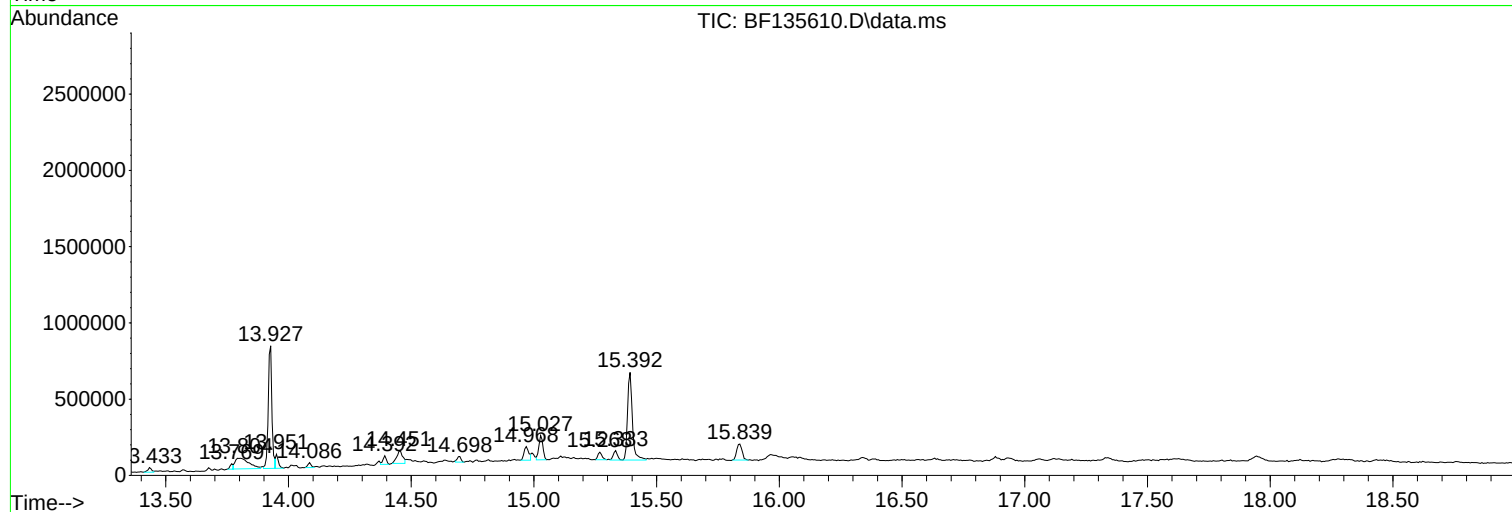
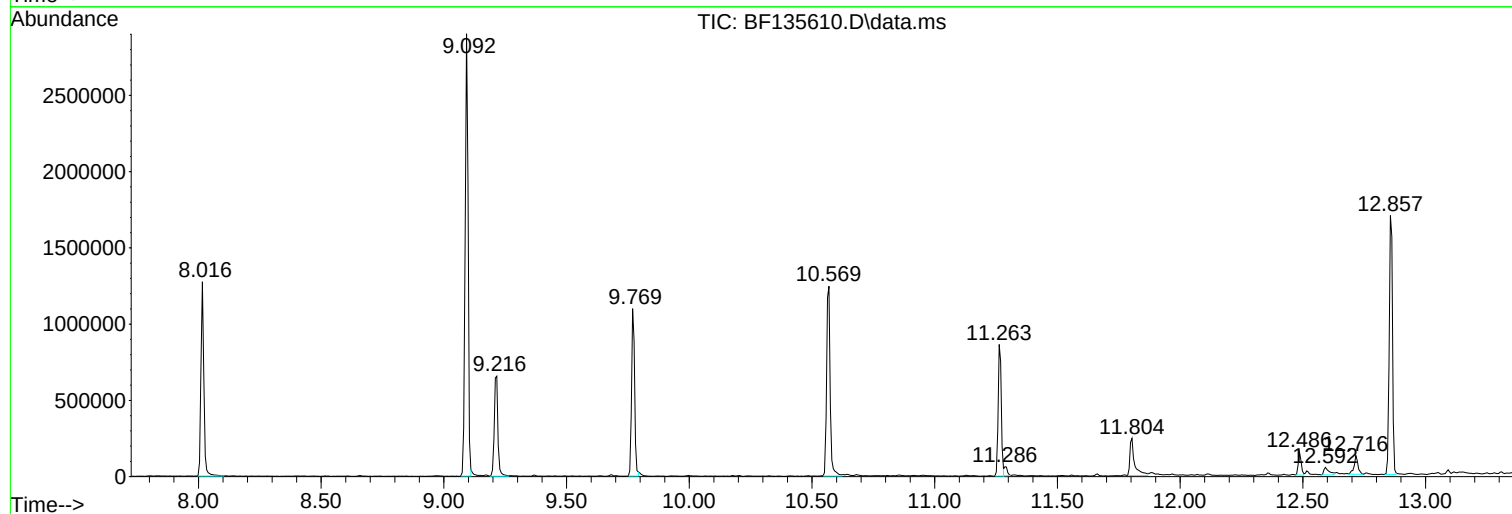
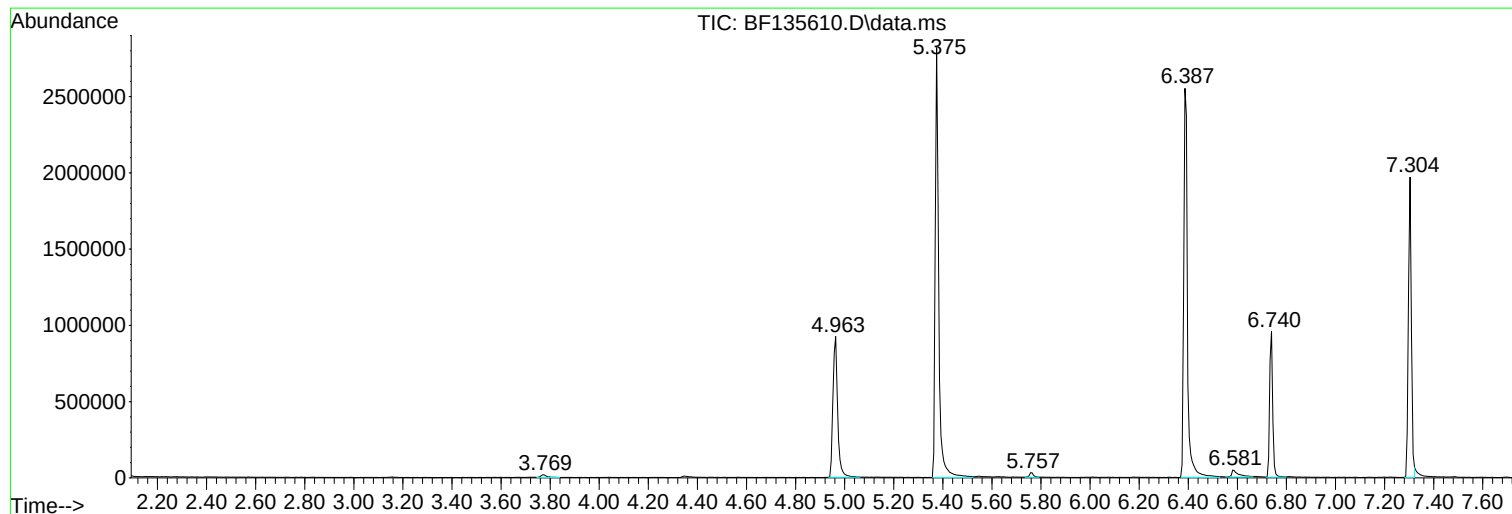
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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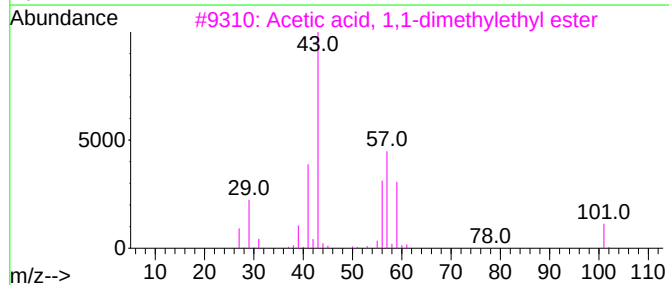
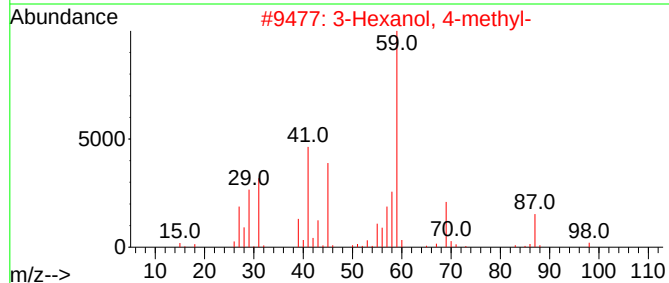
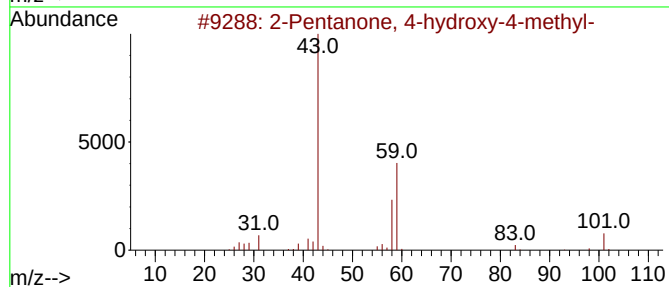
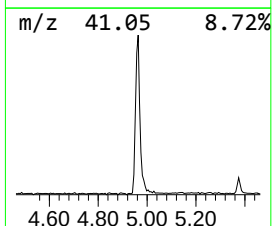
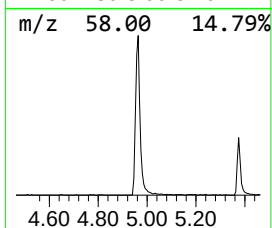
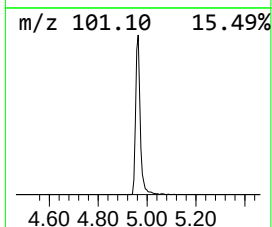
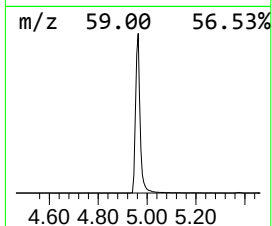
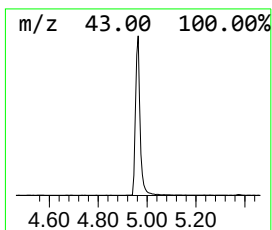
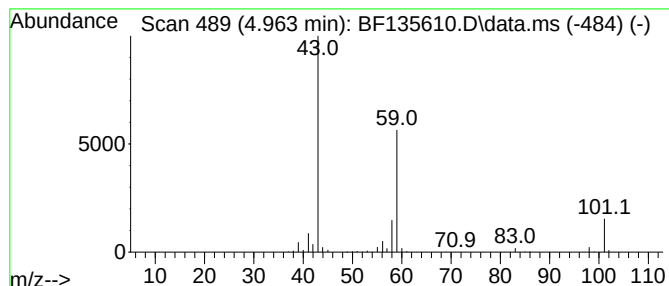
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.963	29.40 ng	1206120	1,4-Dichlorobenzene-d4	6.740

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
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	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



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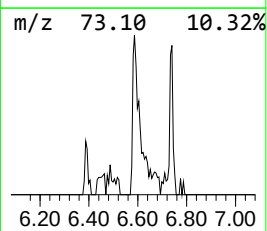
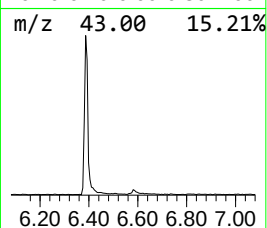
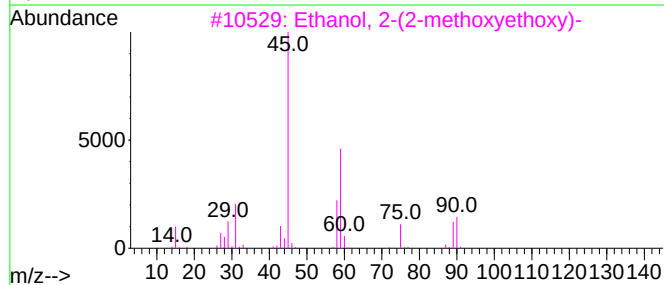
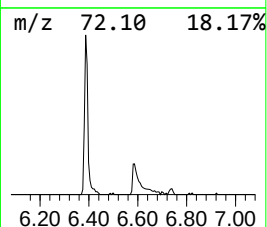
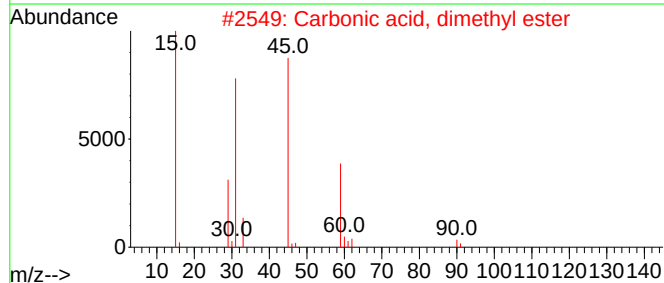
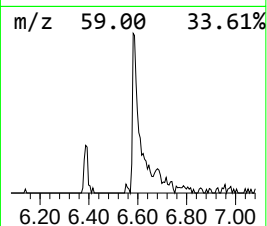
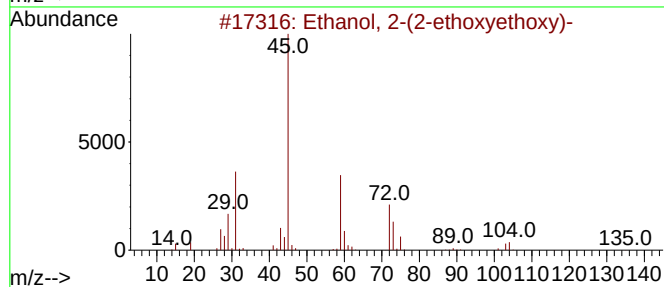
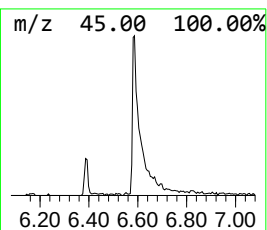
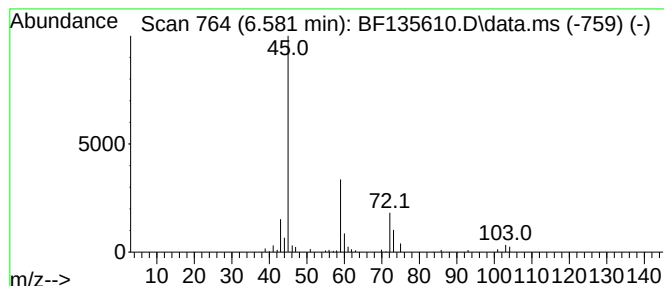
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.581	2.07 ng	84982	1,4-Dichlorobenzene-d4	6.740

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	64
2			Carbonic acid, dimethyl ester	90	C3H6O3	000616-38-6	39
3			Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	38
4			Ethane, 1,2-diethoxy-	118	C6H14O2	000629-14-1	38
5			Diethyl carbitol	162	C8H18O3	000112-36-7	38



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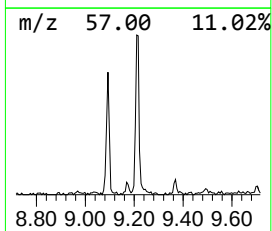
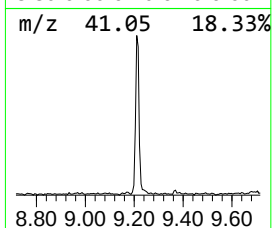
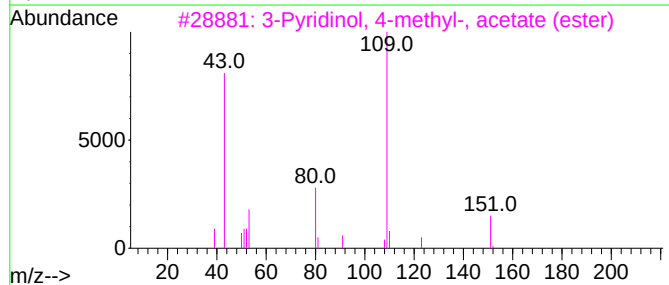
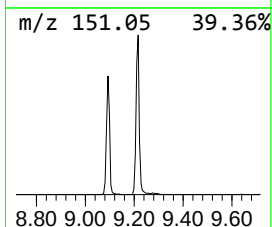
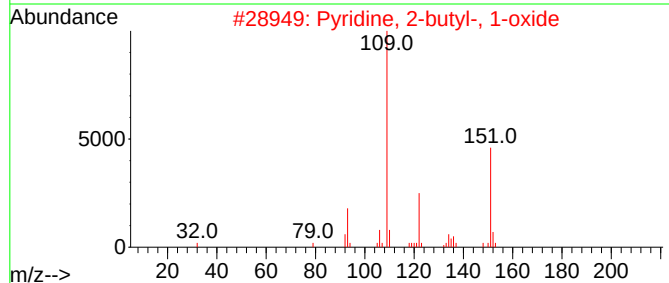
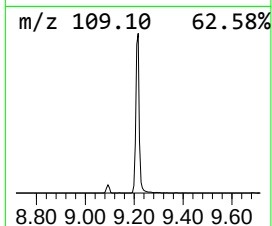
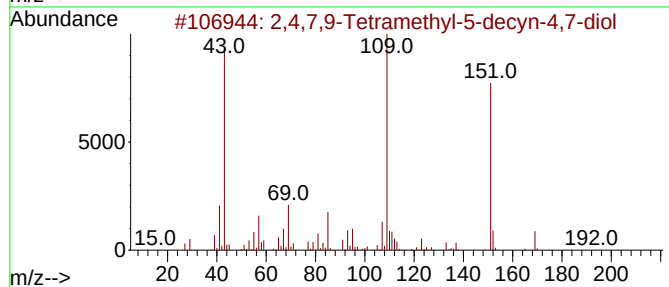
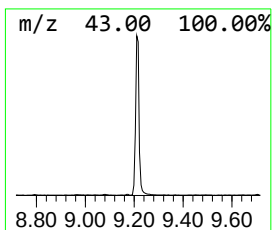
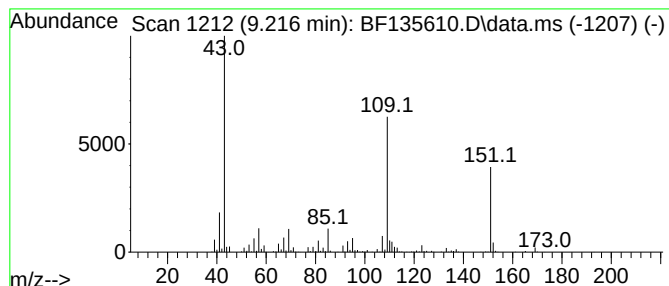
Instrument :
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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.216	14.08 ng	666009	Acenaphthene-d10	9.769	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	86
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	59
3	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	50
4	Metacetamol	151	C8H9NO2	000621-42-1	50
5	Cyclohexanol, 3,3,5-trimethyl-	142	C9H18O	000116-02-9	43



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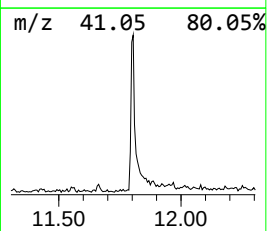
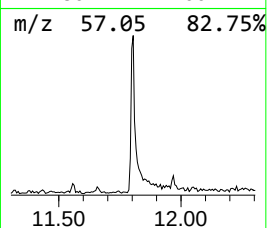
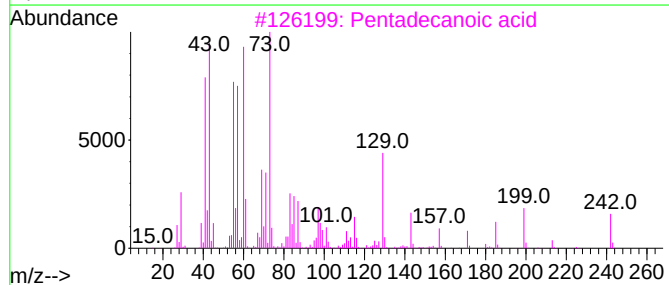
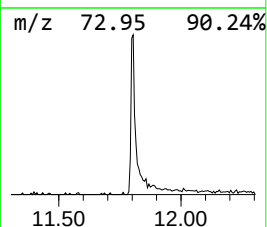
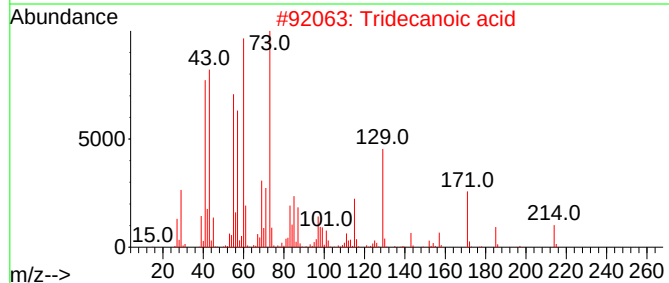
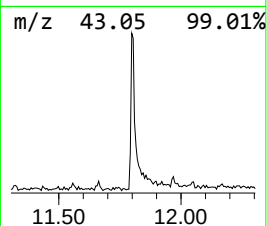
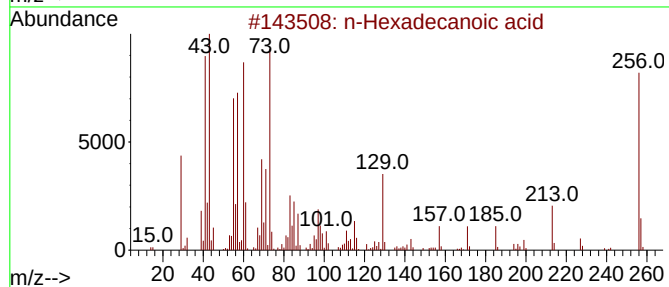
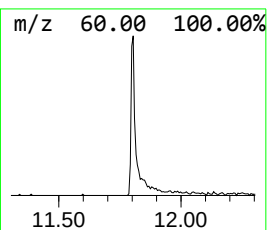
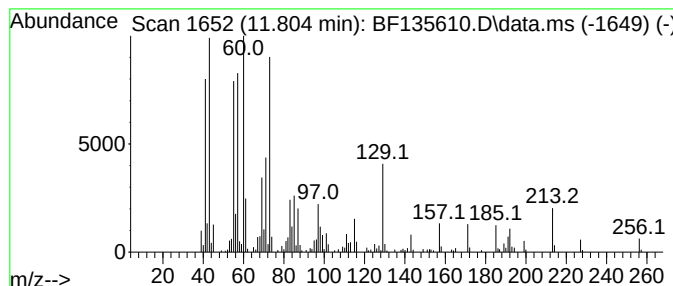
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	8.35 ng	321517	Phenanthrene-d10	11.263

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			n-Decanoic acid	172	C10H20O2	000334-48-5	68



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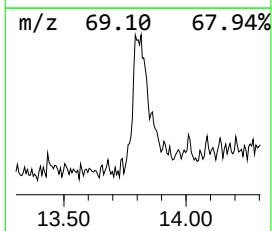
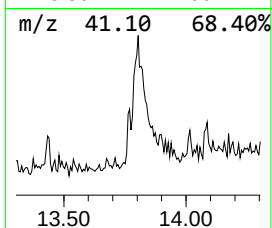
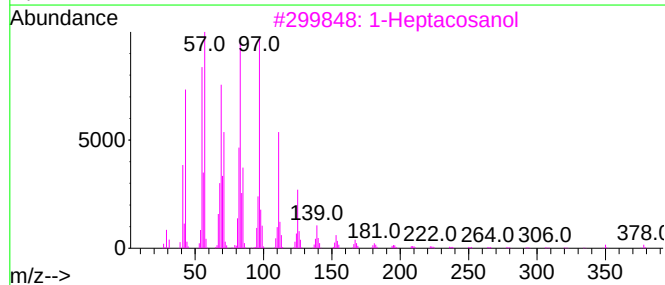
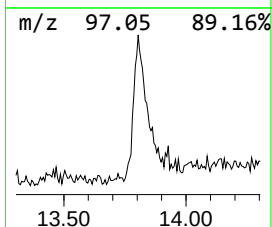
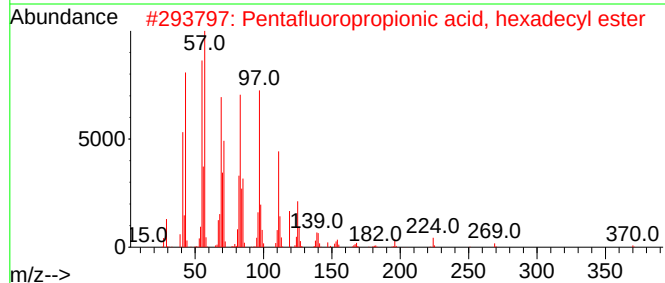
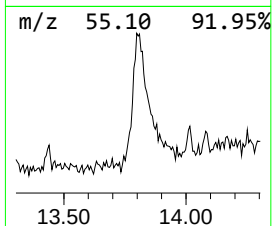
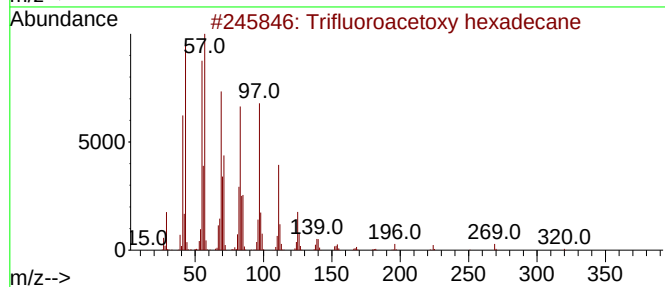
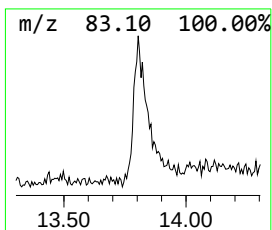
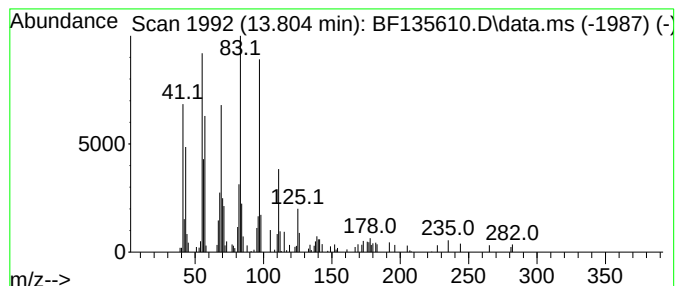
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.804	6.49 ng	272249	Chrysene-d12	13.927

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	74
2			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	74
3			1-Heptacosanol	396	C27H56O	002004-39-9	70
4			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	58
5			1-Octadecanol	270	C18H38O	000112-92-5	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100523\
Data File : BF135610.D
Acq On : 05 Oct 2023 20:47
Operator : CG\JU
Sample : 04714-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

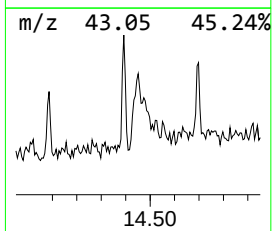
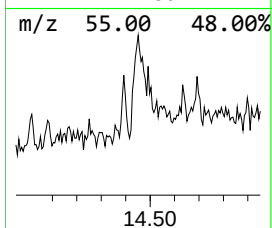
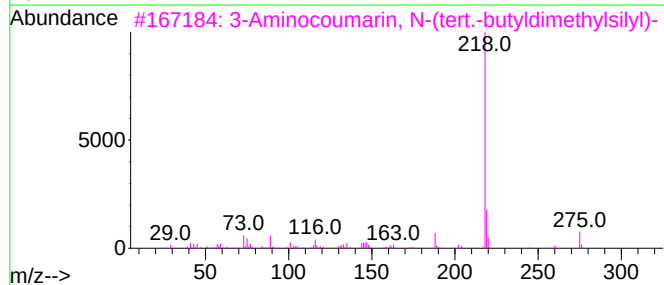
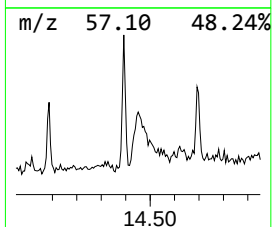
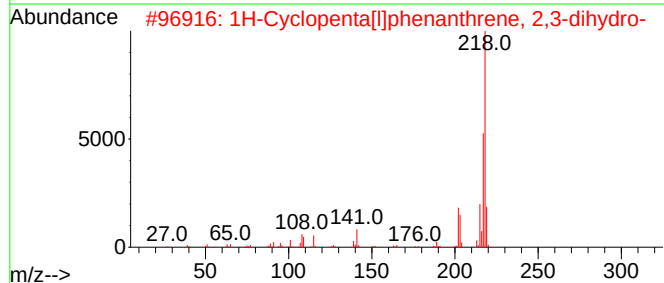
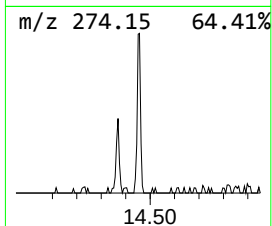
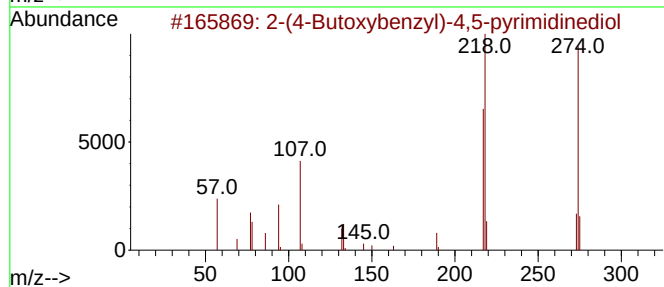
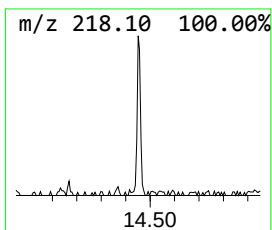
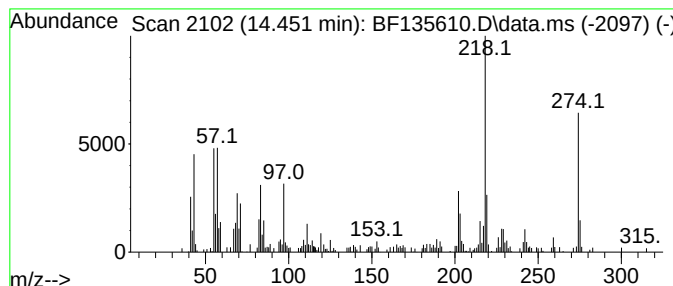
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown14.451 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.451	3.42 ng	143415	Chrysene-d12	13.927

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(4-Butoxybenzyl)-4,5-pyrimidin...	274	C15H18N2O3	1000327-11-0	49		
2	1H-Cyclopenta[l]phenanthrene, 2,...	218	C17H14	000723-98-8	45		
3	3-Aminocoumarin, N-(tert.-butyld...	275	C15H21NO2Si	1000451-95-2	43		
4	9-Phenyl-5H-benzocycloheptene	218	C17H14	138089-71-1	38		
5	4H-Benz[de]anthracene, 5,6-dihydro-	218	C17H14	004389-09-7	35		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100523\
Data File : BF135610.D
Acq On : 05 Oct 2023 20:47
Operator : CG\JU
Sample : 04714-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

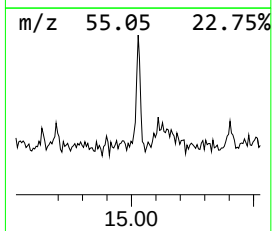
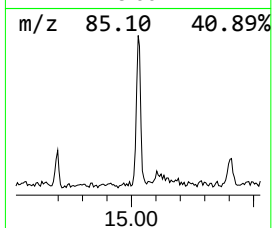
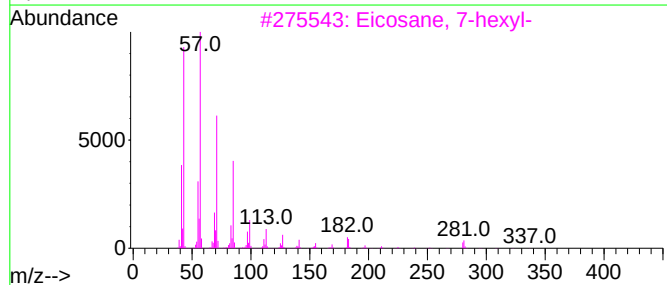
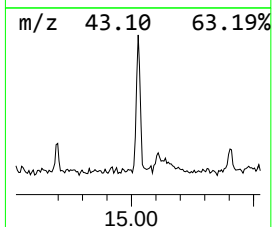
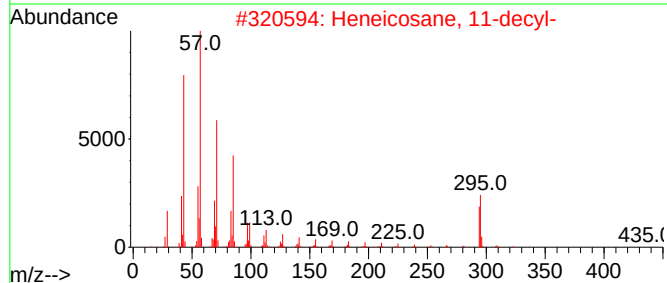
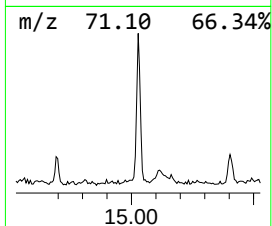
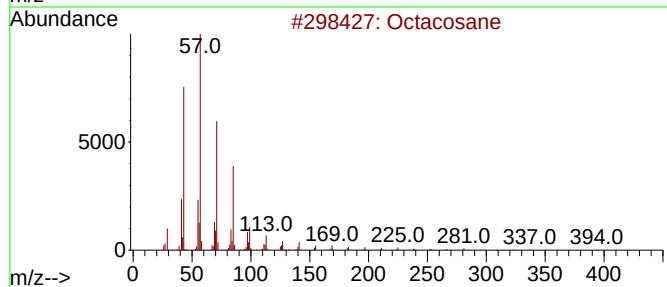
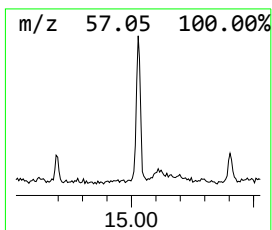
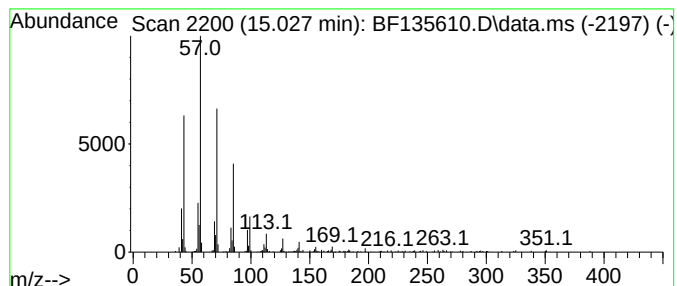
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.027	4.56 ng	179615	Perylene-d12	15.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Heneicosane, 11-decyl-	437	C31H64	055320-06-4	91
3			Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
4			Tetracosane	338	C24H50	000646-31-1	91
5			Hexacosane, 1-iodo-	492	C26H53I	1000406-32-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100523\
Data File : BF135610.D
Acq On : 05 Oct 2023 20:47
Operator : CG\JU
Sample : 04714-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

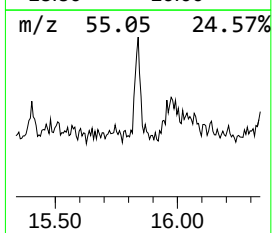
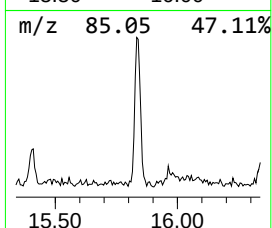
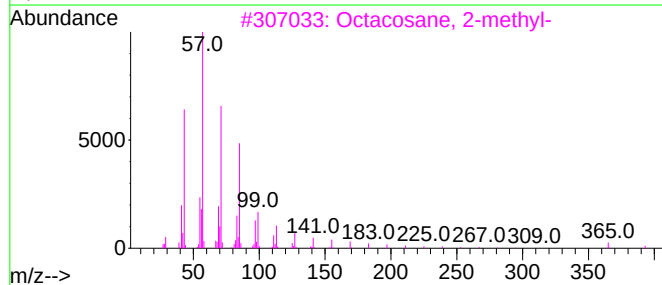
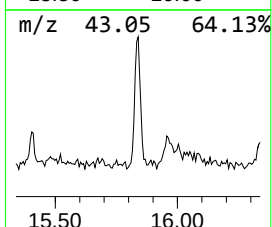
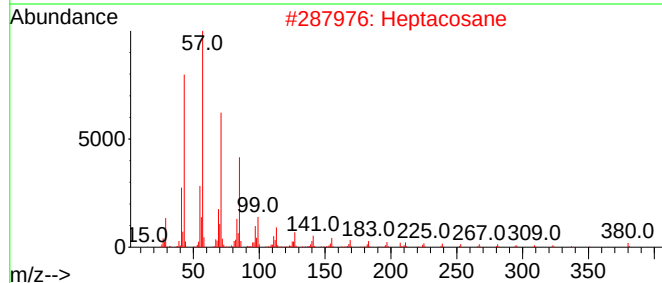
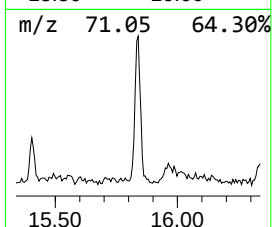
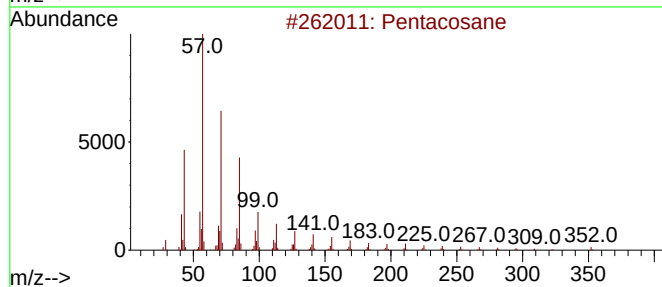
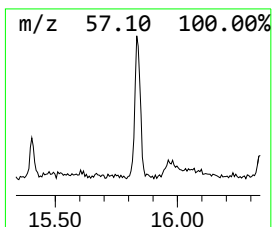
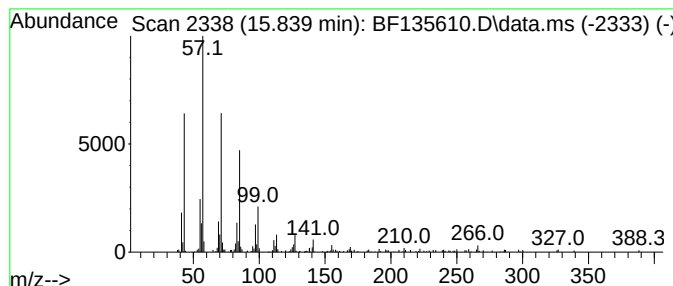
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.839	4.05 ng	159563	Perylene-d12	15.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	87
2			Heptacosane	380	C27H56	000593-49-7	87
3			Octacosane, 2-methyl-	408	C29H60	001560-98-1	83
4			Octacosane	394	C28H58	000630-02-4	81
5			Heneicosane	296	C21H44	000629-94-7	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100523\
Data File : BF135610.D
Acq On : 05 Oct 2023 20:47
Operator : CG\JU
Sample : 04714-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

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
2-Pentanone, 4-...	4.963	29.4	ng	1206120	1	6.740	820392	20.0
Ethanol, 2-(2-e...	6.581	2.1	ng	84982	1	6.740	820392	20.0
2,4,7,9-Tetrame...	9.216	14.1	ng	666009	3	9.769	945813	20.0
n-Hexadecanoic ...	11.804	8.3	ng	321517	4	11.263	769654	20.0
Trifluoroacetox...	13.804	6.5	ng	272249	5	13.927	839099	20.0
unknown14.451	14.451	3.4	ng	143415	5	13.927	839099	20.0
Octacosane	15.027	4.6	ng	179615	6	15.392	788165	20.0
Pentacosane	15.839	4.0	ng	159563	6	15.392	788165	20.0