

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090624\
 Data File : BF139276.D
 Acq On : 06 Sep 2024 14:32
 Operator : RC/JU
 Sample : P3861-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DN-B-37

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-BF090424.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139276.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	9	17	25	rVB	1351829	2098928	79.99%	9.940%
2	5.104	503	512	518	rVB	123564	192327	7.33%	0.911%
3	5.504	574	580	585	rBV	1687746	2215205	84.42%	10.490%
4	6.510	745	751	756	rBV	1747230	2359822	89.93%	11.175%
5	6.887	810	815	820	rVB	589266	706270	26.92%	3.345%
6	7.445	900	910	915	rBV	1143231	1522767	58.03%	7.211%
7	8.169	1020	1033	1040	rBV	723541	939007	35.78%	4.447%
8	8.481	1076	1086	1089	rBV6	23990	61464	2.34%	0.291%
9	8.586	1101	1104	1115	rVB	29475	49137	1.87%	0.233%
10	8.757	1129	1133	1137	rBV	86008	102939	3.92%	0.487%
11	9.045	1178	1182	1186	rBV3	14561	29038	1.11%	0.138%
12	9.245	1210	1216	1221	rBV	2120591	2624047	100.00%	12.427%
13	9.322	1225	1229	1235	rVV	58884	75825	2.89%	0.359%
14	9.922	1326	1331	1336	rBV	694113	870916	33.19%	4.124%
15	10.639	1445	1453	1458	rBV	147645	189486	7.22%	0.897%
16	10.710	1460	1465	1470	rBV	1044366	1296592	49.41%	6.140%
17	11.145	1535	1539	1546	rVB3	18944	31031	1.18%	0.147%
18	11.410	1579	1584	1592	rBV	614965	835389	31.84%	3.956%
19	11.580	1609	1613	1618	rVB2	19550	29831	1.14%	0.141%
20	11.904	1664	1668	1670	rBV3	45973	67848	2.59%	0.321%
21	11.939	1670	1674	1681	rVV	440906	590647	22.51%	2.797%
22	12.622	1786	1790	1801	rBV	144535	302792	11.54%	1.434%
23	12.722	1802	1807	1810	rVV3	123869	210563	8.02%	0.997%
24	12.751	1810	1812	1819	rVV	122278	178639	6.81%	0.846%
25	12.810	1819	1822	1825	rVV	38358	52511	2.00%	0.249%
26	12.851	1825	1829	1836	rVB	107948	163637	6.24%	0.775%
27	12.998	1849	1854	1862	rVB	1539793	1961656	74.76%	9.290%
28	13.904	2004	2008	2017	rBV2	148856	253768	9.67%	1.202%
29	14.051	2028	2033	2040	rVB2	413331	626528	23.88%	2.967%
30	15.180	2222	2225	2237	rVB2	116329	186500	7.11%	0.883%
31	15.527	2280	2284	2288	rBV	203205	291386	11.10%	1.380%

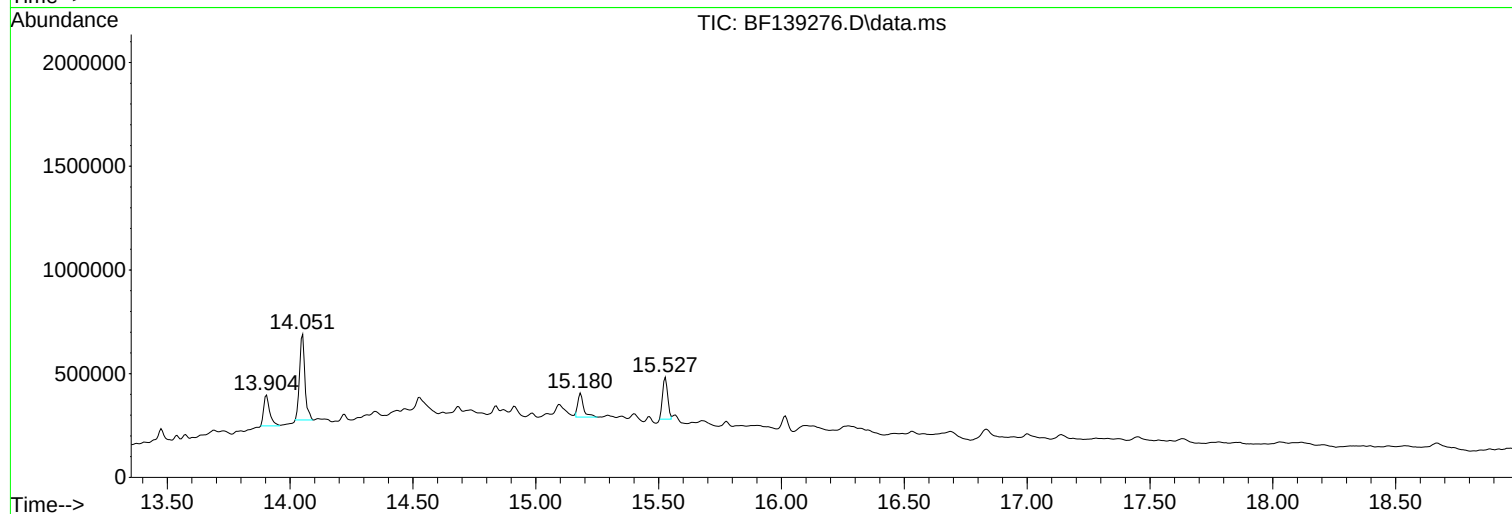
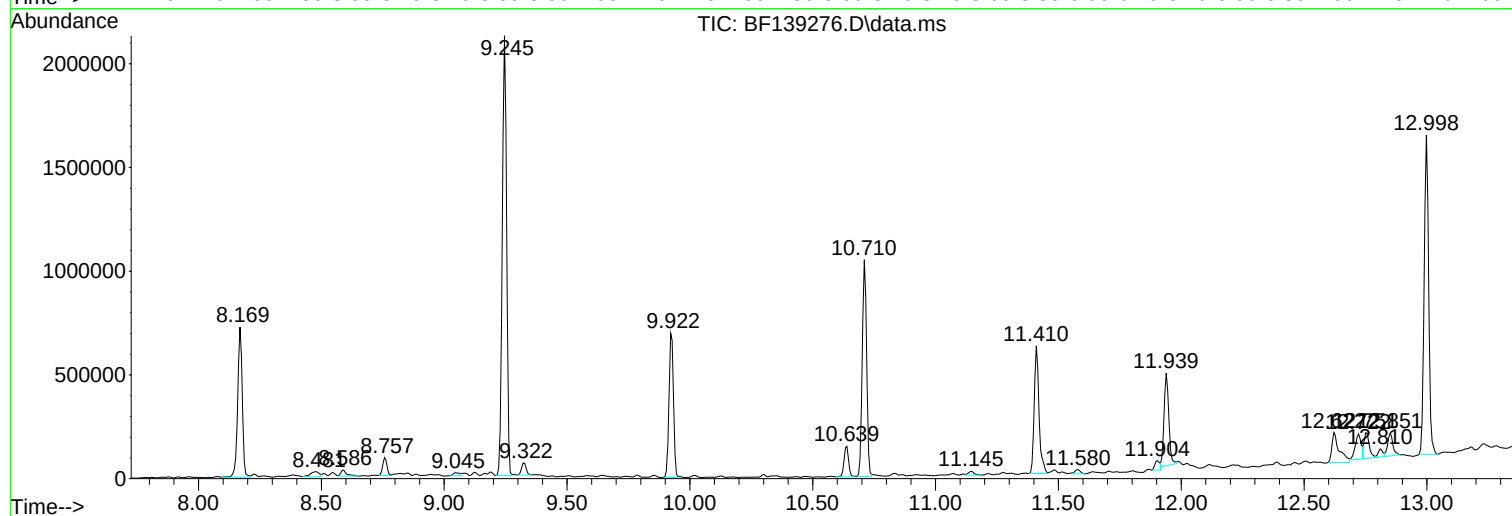
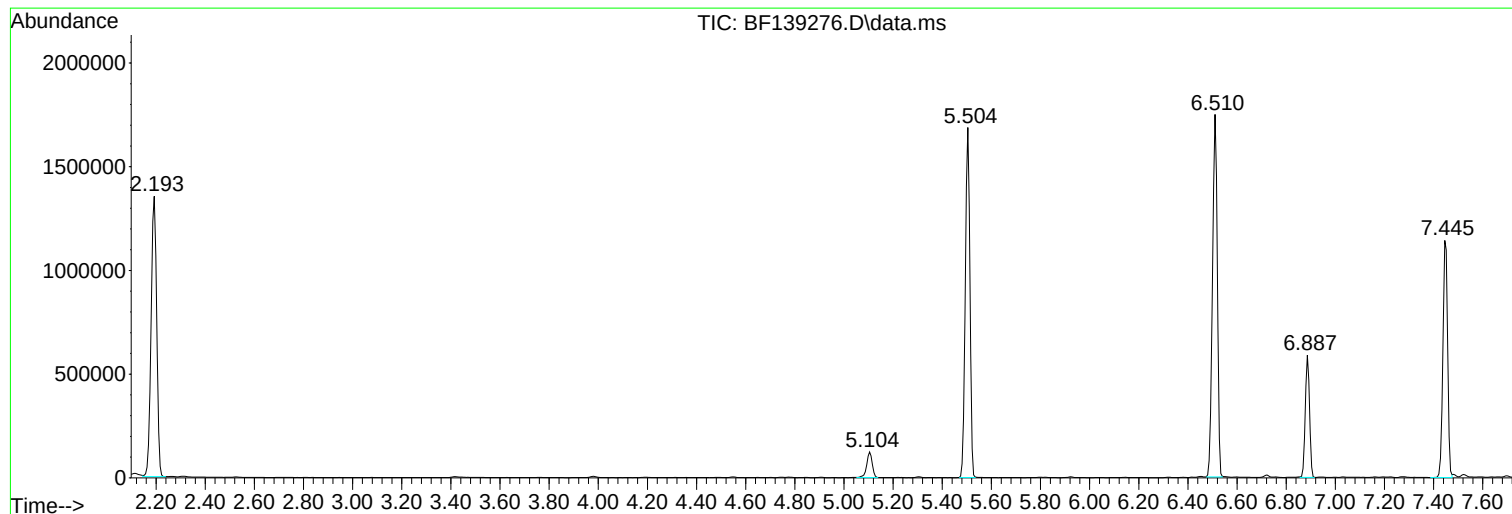
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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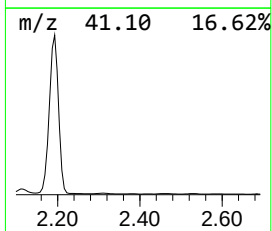
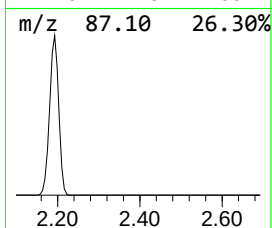
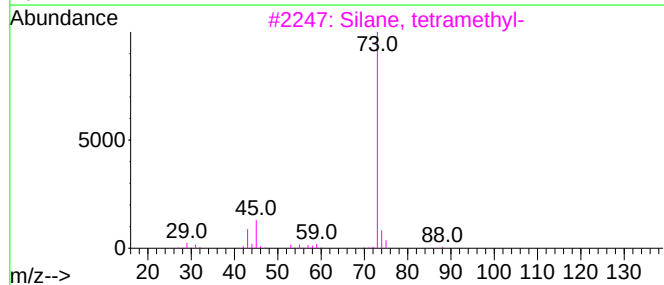
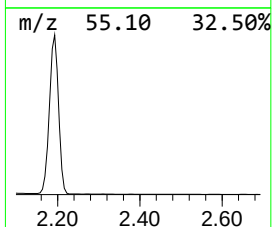
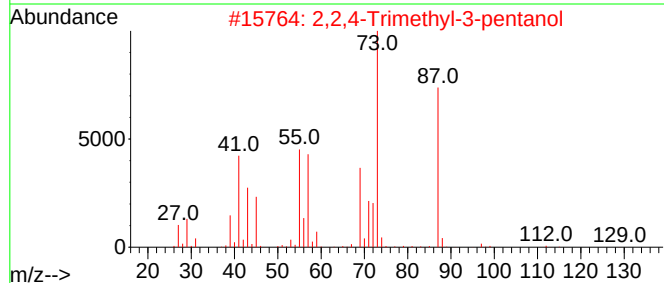
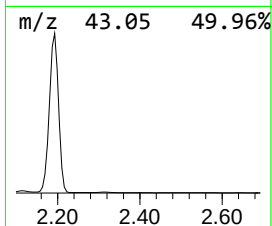
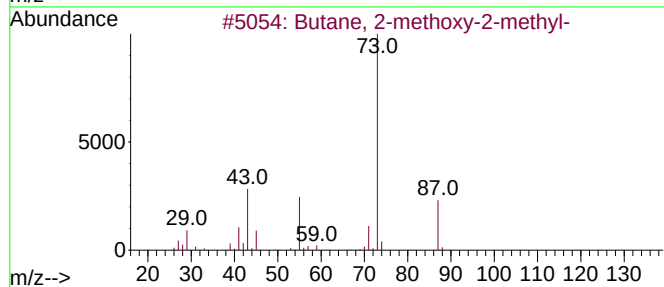
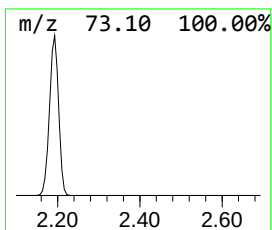
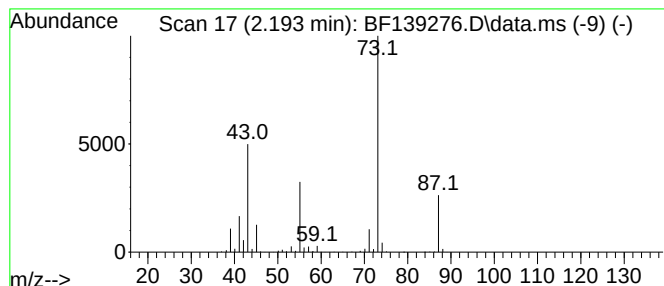
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.193	59.44 ng	2098930	1,4-Dichlorobenzene-d4	6.887

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			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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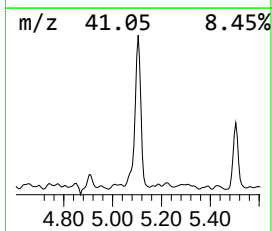
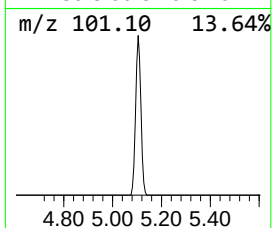
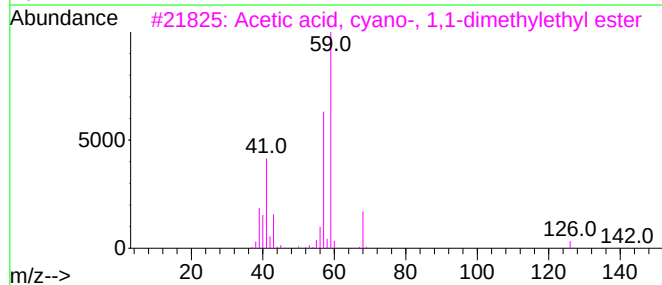
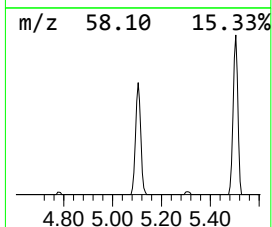
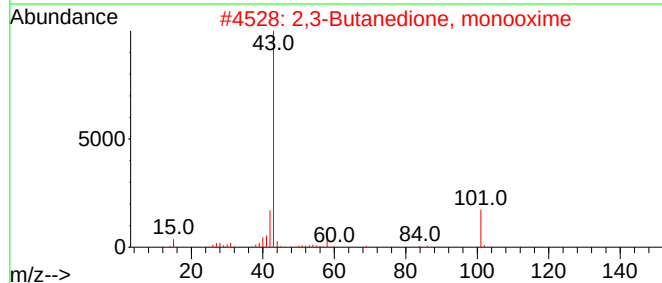
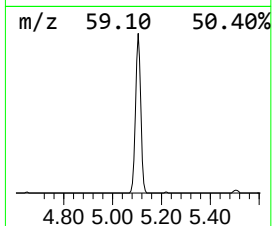
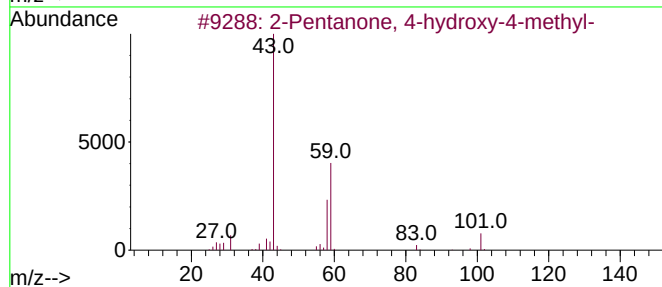
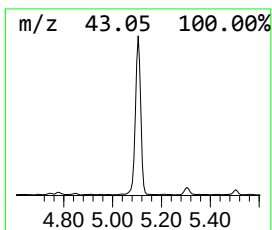
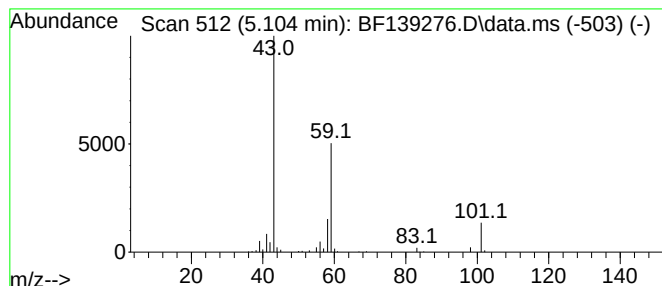
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	5.45 ng	192327	1,4-Dichlorobenzene-d4	6.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			5-Aminovaleric acid	117	C5H11NO2	000660-88-8	9



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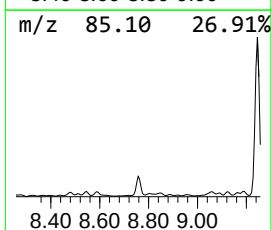
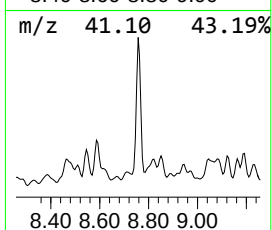
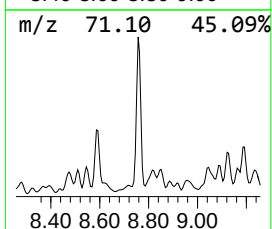
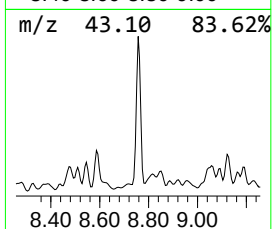
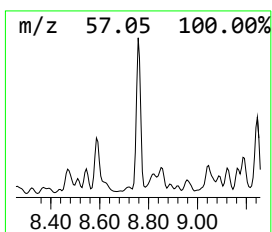
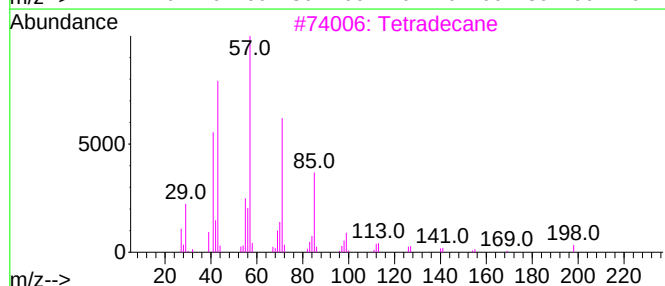
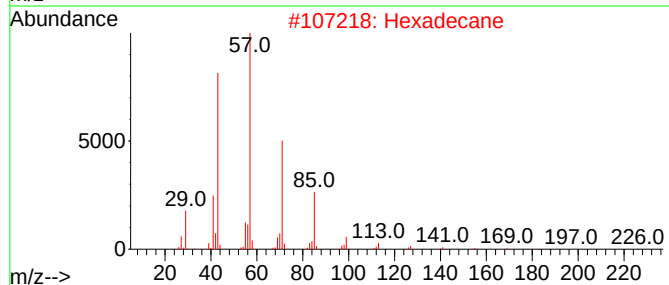
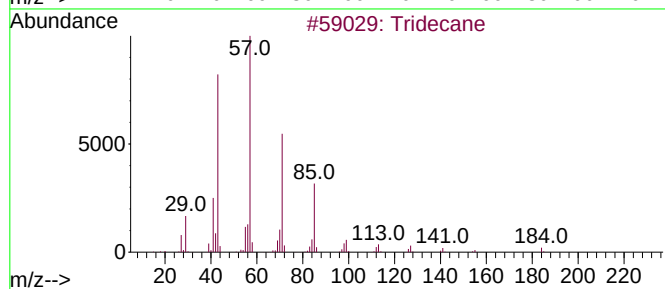
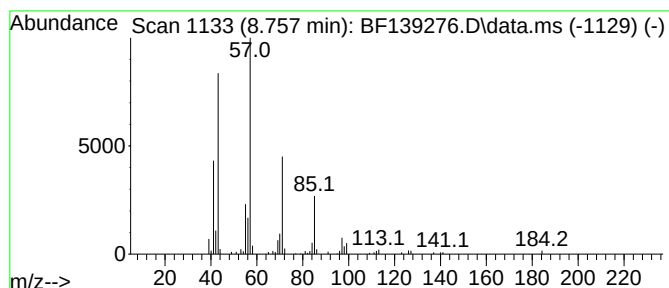
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Tridecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.757	2.19 ng	102939	Naphthalene-d8	8.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	90
2			Hexadecane	226	C16H34	000544-76-3	87
3			Tetradecane	198	C14H30	000629-59-4	86
4			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	72
5			Heptadecane	240	C17H36	000629-78-7	72



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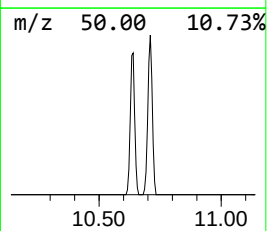
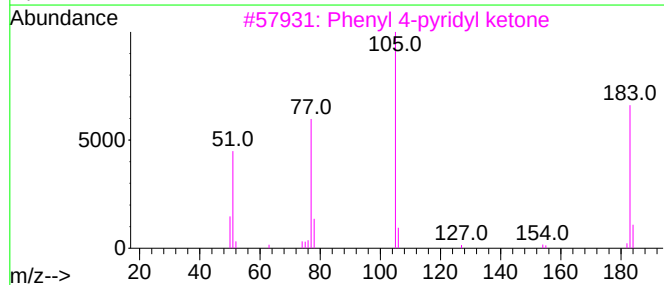
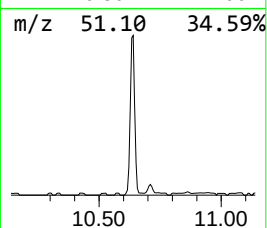
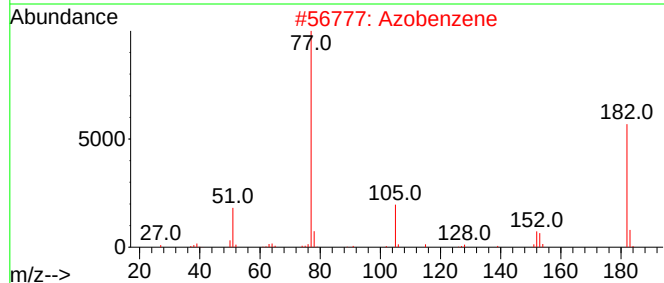
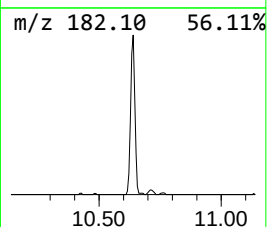
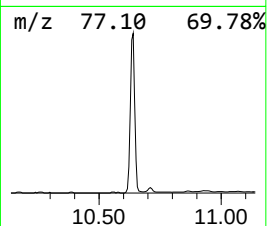
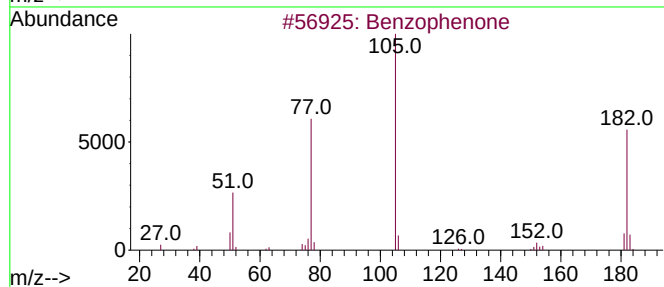
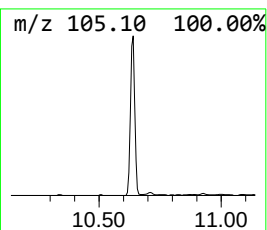
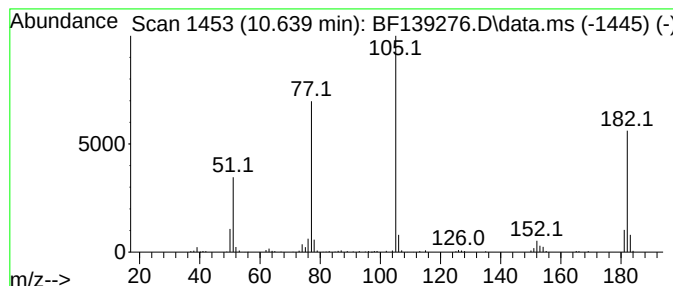
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Benzophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.639	4.35 ng	189486	Acenaphthene-d10	9.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene	182	C12H10N2	000103-33-3	52
3			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	50
4			Ethanone, 2,2-dihydroxy-1-phenyl-	152	C8H8O3	001075-06-5	47
5			Benzoic acid, 2-(benzoylthio)thi...	341	C17H11NO3S2	1000258-72-7	47



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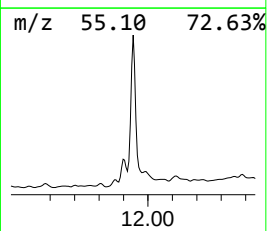
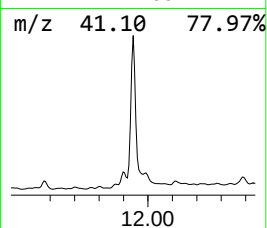
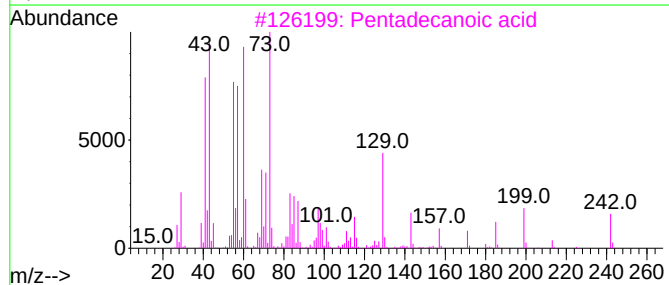
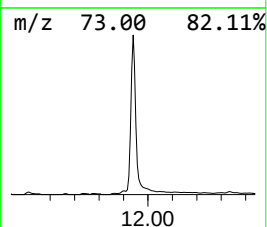
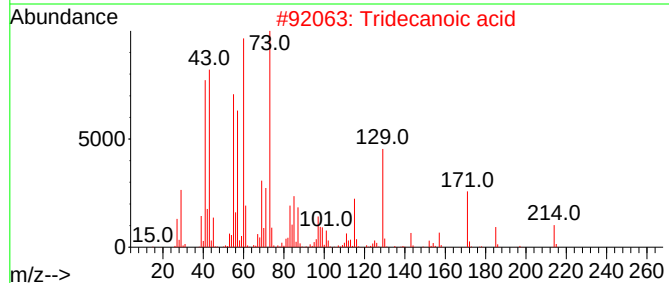
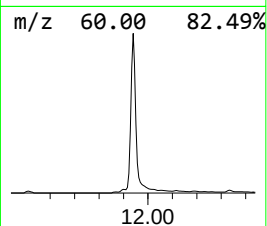
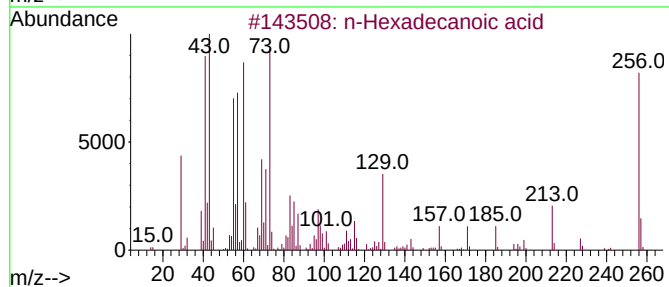
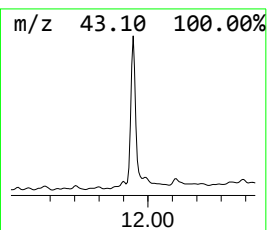
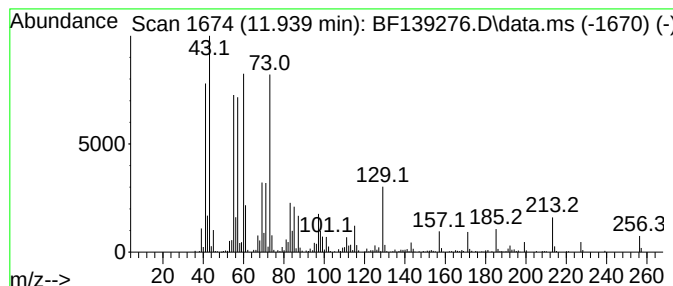
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.939	14.14 ng	590647	Phenanthrene-d10		11.410	
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	95
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	87
5	Undecanoic acid		186	C11H22O2	000112-37-8	62



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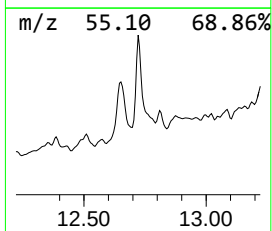
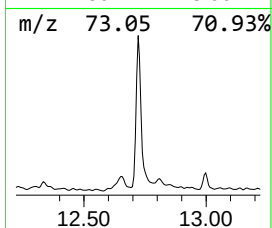
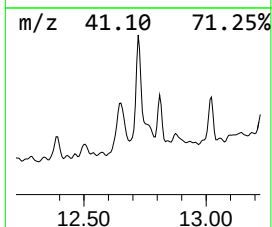
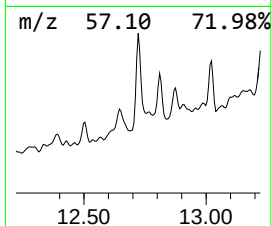
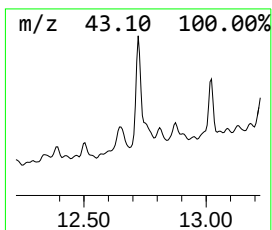
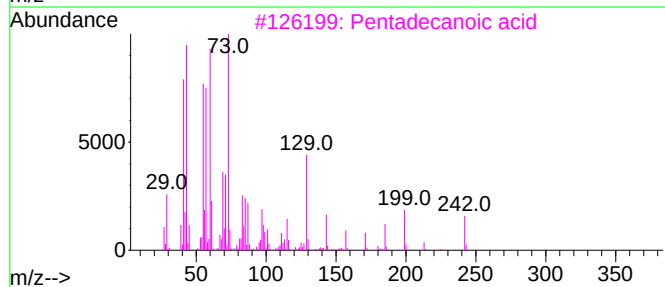
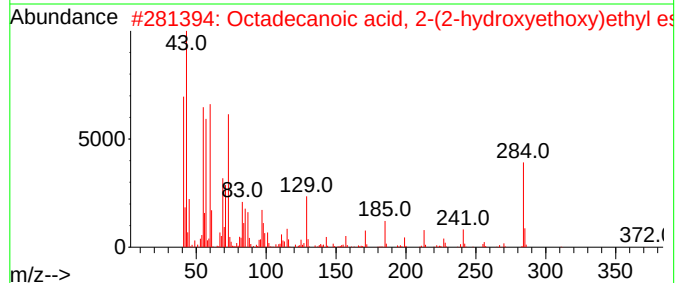
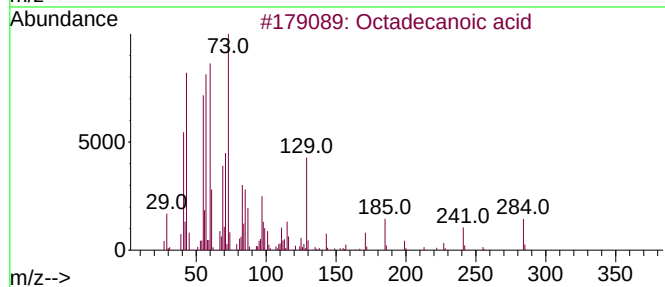
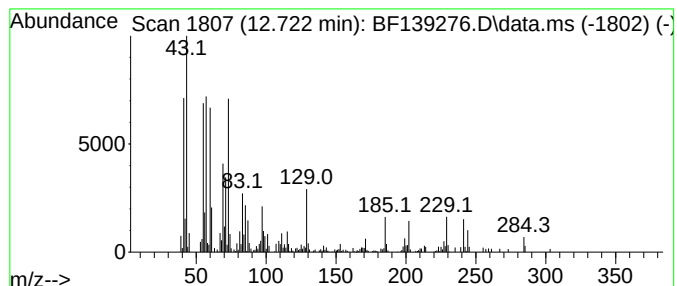
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.722	5.04 ng	210563	Phenanthrene-d10	11.410

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	95
2		Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	68
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	58
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5		Tridecanoic acid	214	C13H26O2	000638-53-9	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090624\
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Acq On : 06 Sep 2024 14:32
Operator : RC/JU
Sample : P3861-01
Misc :
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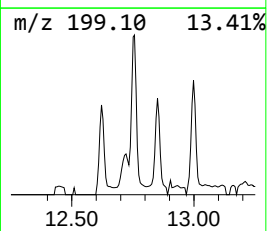
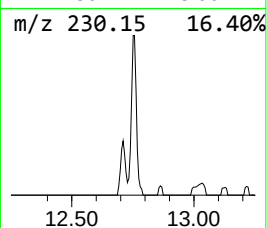
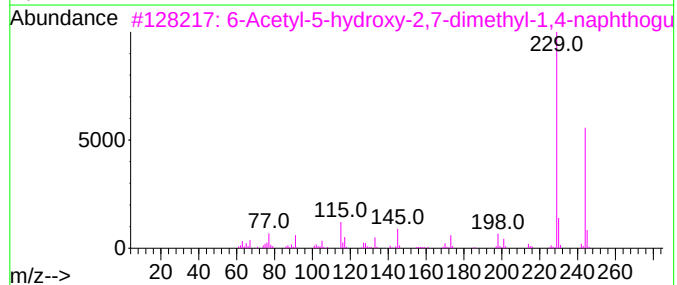
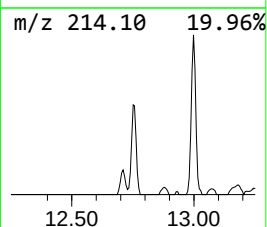
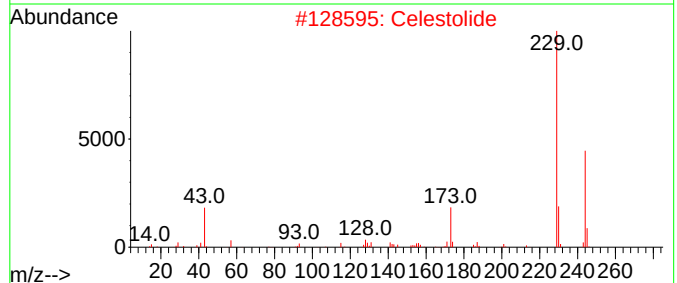
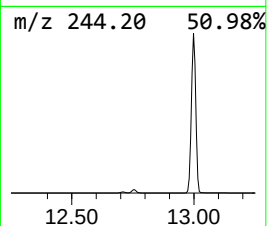
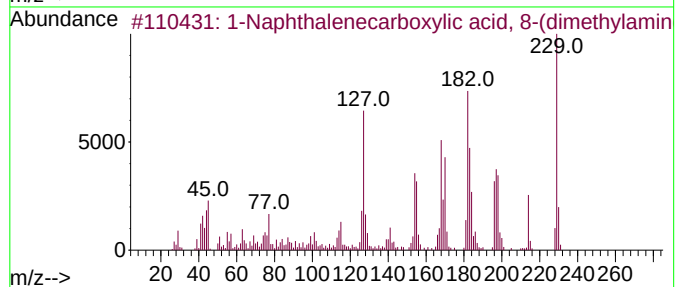
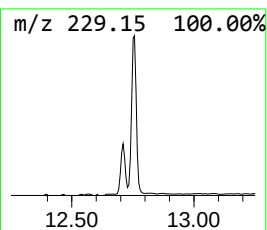
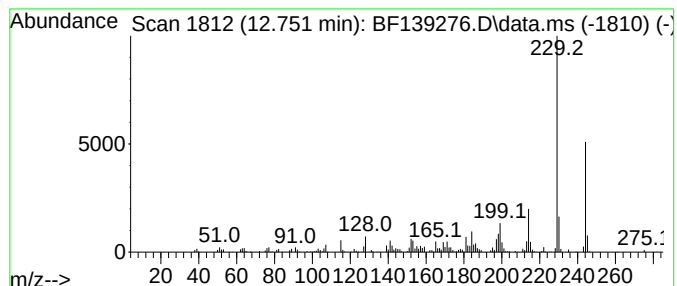
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DN-B-37

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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 1-Naphthalenecarboxylic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.751	5.70 ng	178639	Chrysene-d12	14.051	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Naphthalenecarboxylic acid, 8-...	229	C14H15NO2	069674-55-1	86
2	Celestolide	244	C17H24O	013171-00-1	70
3	6-Acetyl-5-hydroxy-2,7-dimethyl-...	244	C14H12O4	001086-07-3	64
4	2-Propenoic acid, 2-cyano-3-[4-(...	244	C14H16N2O2	1000115-72-8	62
5	Cyclopentanone, tetrakis(1-methy...	244	C17H24O	096446-08-1	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090624\
Data File : BF139276.D
Acq On : 06 Sep 2024 14:32
Operator : RC/JU
Sample : P3861-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DN-B-37

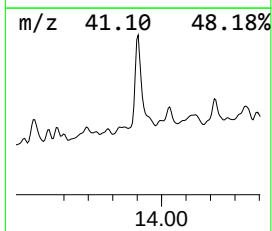
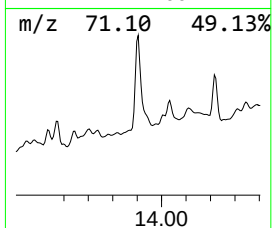
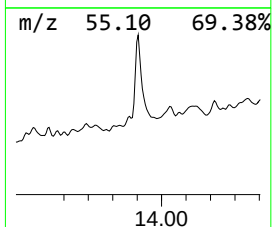
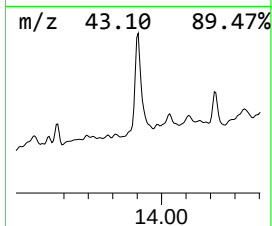
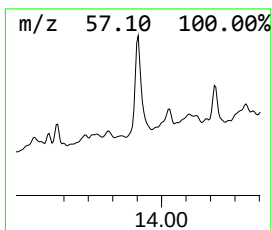
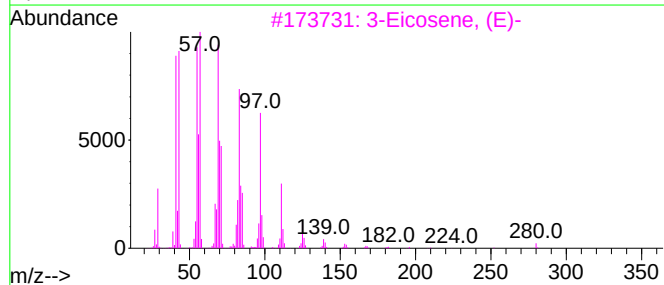
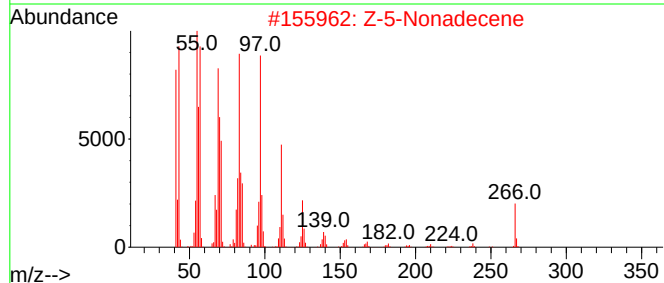
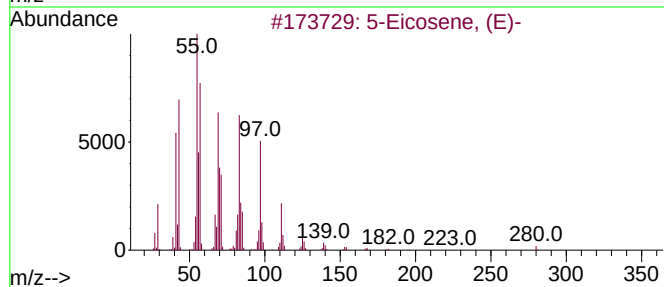
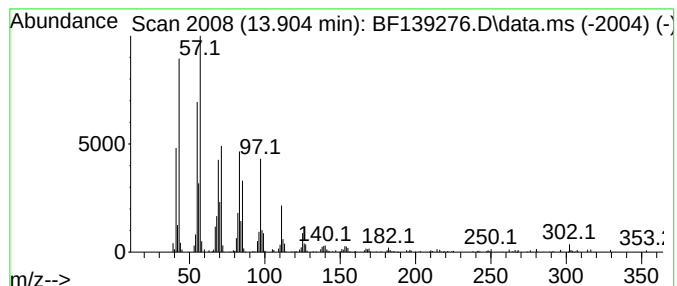
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	8.10 ng	253768	Chrysene-d12	14.051

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Eicosene, (E)-	280	C20H40	074685-30-6	98
2		Z-5-Nonadecene	266	C19H38	1000131-11-8	97
3		3-Eicosene, (E)-	280	C20H40	074685-33-9	93
4		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
5		Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090624\
Data File : BF139276.D
Acq On : 06 Sep 2024 14:32
Operator : RC/JU
Sample : P3861-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DN-B-37

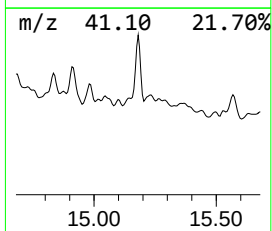
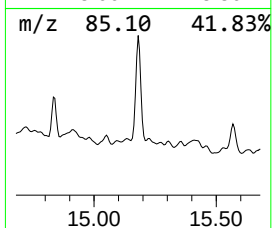
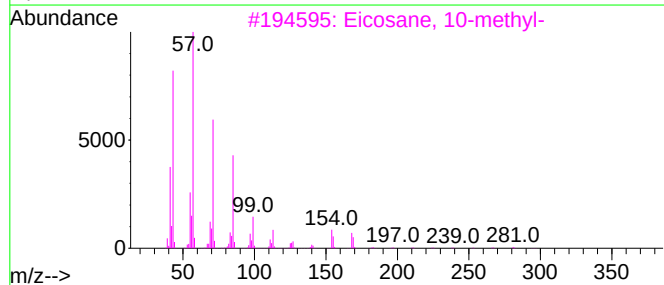
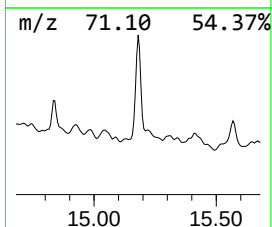
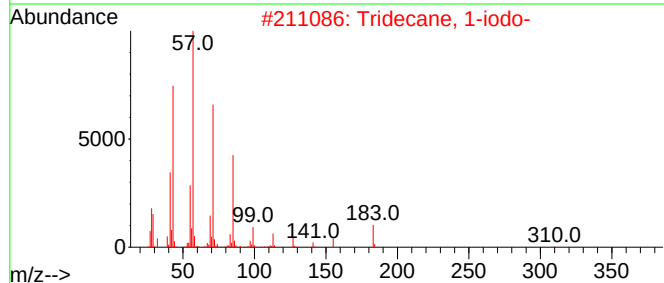
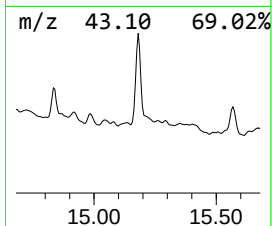
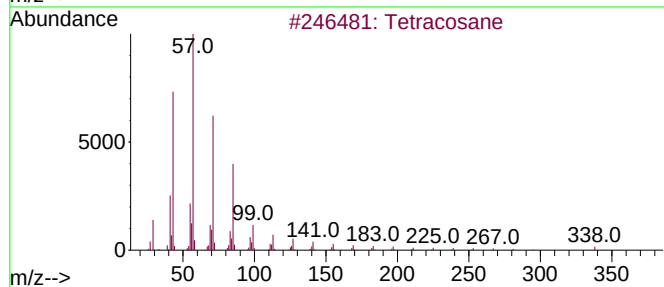
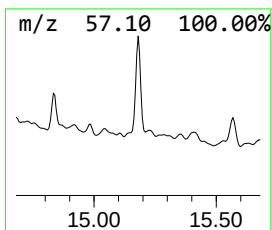
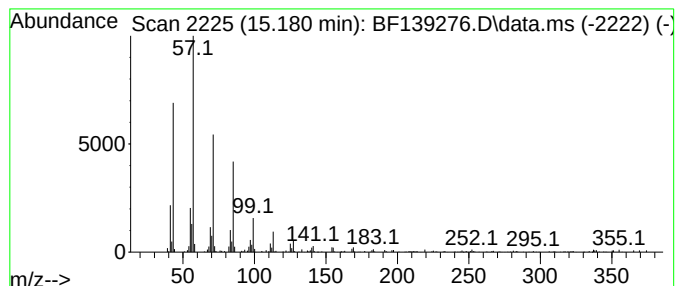
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetracosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.180	12.80 ng	186500	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	93
2			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	93
3			Eicosane, 10-methyl-	296	C21H44	054833-23-7	91
4			Eicosane	282	C20H42	000112-95-8	90
5			1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090624\
Data File : BF139276.D
Acq On : 06 Sep 2024 14:32
Operator : RC/JU
Sample : P3861-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DN-B-37

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.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...	2.193	59.4	ng	2098930	1	6.887	706270	20.0
2-Pentanone, 4-...	5.104	5.5	ng	192327	1	6.887	706270	20.0
Tridecane	8.757	2.2	ng	102939	2	8.169	939007	20.0
Benzophenone	10.639	4.3	ng	189486	3	9.922	870916	20.0
n-Hexadecanoic ...	11.939	14.1	ng	590647	4	11.410	835389	20.0
Octadecanoic acid	12.722	5.0	ng	210563	4	11.410	835389	20.0
1-Naphthaleneca...	12.751	5.7	ng	178639	5	14.051	626528	20.0
5-Eicosene, (E)-	13.904	8.1	ng	253768	5	14.051	626528	20.0
Tetracosane	15.180	12.8	ng	186500	6	15.527	291386	20.0