

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081721\
 Data File : BF125077.D
 Acq On : 17 Aug 2021 20:01
 Operator : JU/CG
 Sample : M3428-17
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-06-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-BF081721.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125077.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.228	17	24	33	rVB	1490994	1926590	45.81%	5.715%
2	3.451	229	232	239	rBV	20994	49949	1.19%	0.148%
3	5.145	510	520	525	rBV	207889	278317	6.62%	0.826%
4	5.534	581	586	589	rBV	3897718	3896613	92.65%	11.559%
5	6.534	750	756	759	rBV	3651104	4102331	97.54%	12.169%
6	6.734	788	790	797	rBV	52870	50535	1.20%	0.150%
7	6.916	818	821	825	rVB	1143471	993402	23.62%	2.947%
8	7.481	912	917	920	rBV	2823172	2617412	62.24%	7.764%
9	8.098	1018	1022	1025	rBV	1852059	1479242	35.17%	4.388%
10	8.204	1035	1040	1043	rVB	1419340	1295720	30.81%	3.844%
11	9.275	1217	1222	1226	rBV	4130999	4033296	95.90%	11.964%
12	9.386	1237	1241	1244	rVB	57959	45299	1.08%	0.134%
13	9.533	1263	1266	1269	rBV	71544	49924	1.19%	0.148%
14	9.957	1334	1338	1341	rBV	1664763	1321963	31.43%	3.921%
15	10.745	1467	1472	1475	rBV	2864389	2581980	61.39%	7.659%
16	11.445	1587	1591	1594	rBV	1567823	1377097	32.74%	4.085%
17	11.833	1653	1657	1660	rBV	207002	155668	3.70%	0.462%
18	11.963	1674	1679	1684	rBV	202046	205023	4.87%	0.608%
19	12.539	1771	1777	1785	rBV	125180	115658	2.75%	0.343%
20	12.745	1808	1812	1816	rBV2	80873	99315	2.36%	0.295%
21	13.033	1856	1861	1864	rBV	4706340	4205676	100.00%	12.476%
22	13.921	2008	2012	2022	rBV	674650	682001	16.22%	2.023%
23	14.080	2031	2039	2043	rBV	1220329	1098147	26.11%	3.258%
24	14.557	2116	2120	2127	rBV	82554	104379	2.48%	0.310%
25	15.221	2229	2233	2243	rVB	58235	92313	2.19%	0.274%
26	15.574	2288	2293	2298	rBV	558349	702470	16.70%	2.084%
27	16.068	2372	2377	2380	rBV	46169	65098	1.55%	0.193%
28	16.115	2380	2385	2393	rVB3	48149	85639	2.04%	0.254%

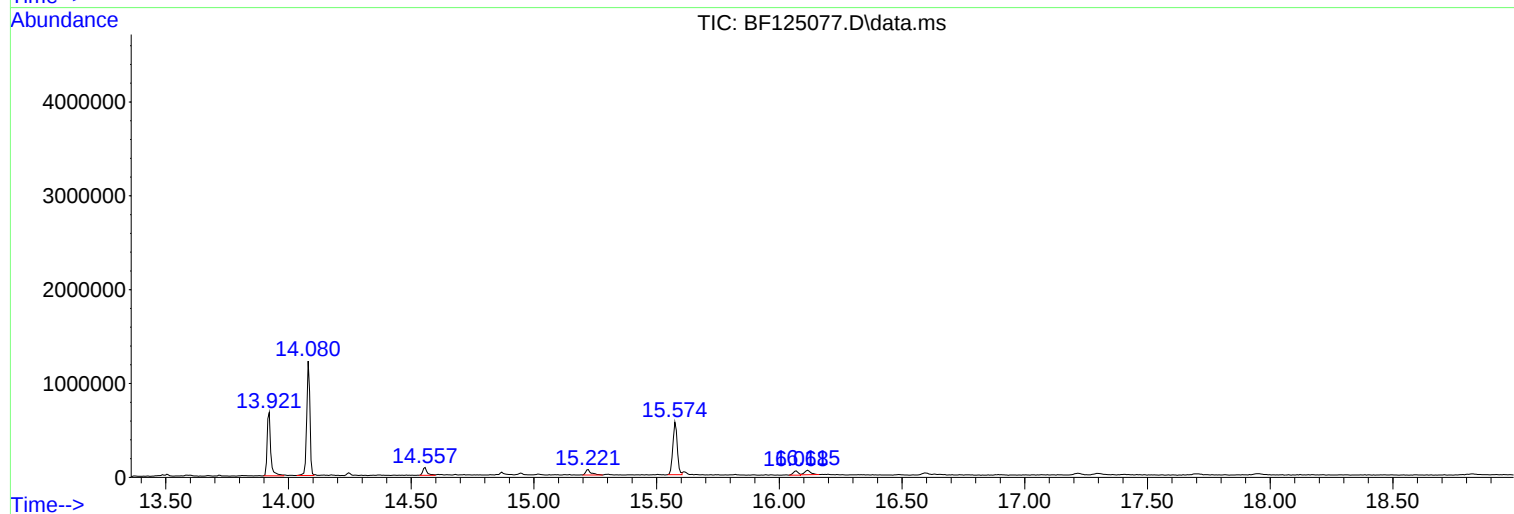
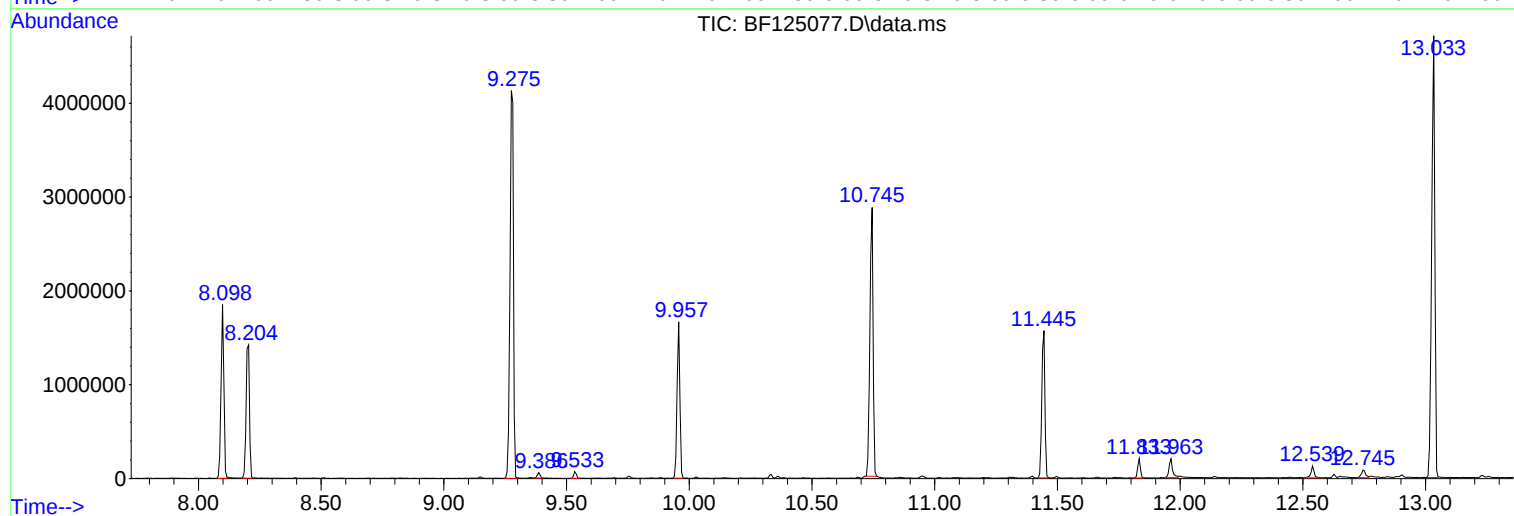
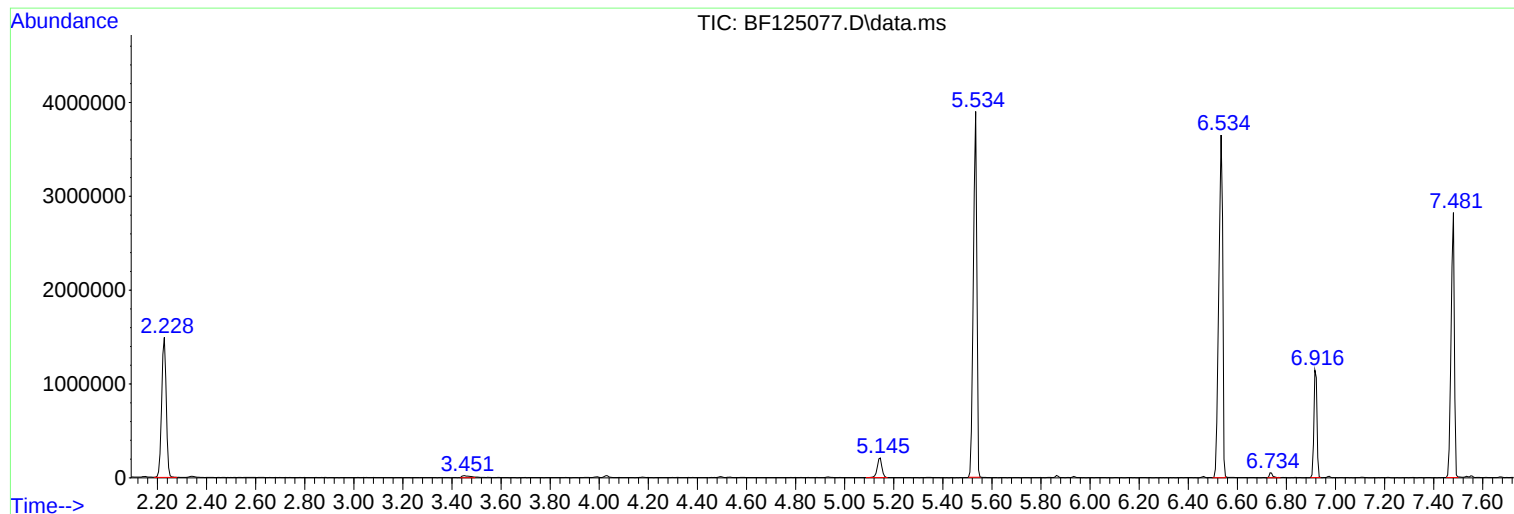
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Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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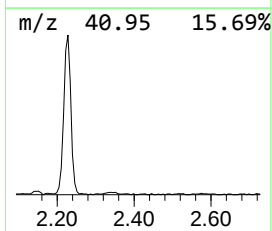
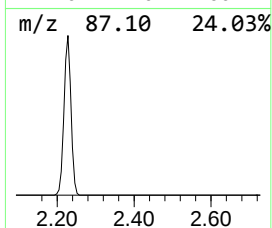
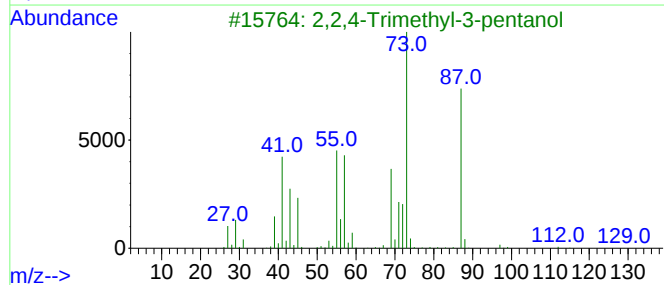
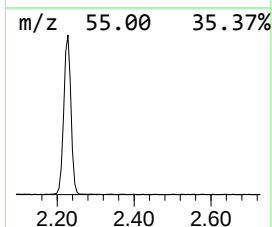
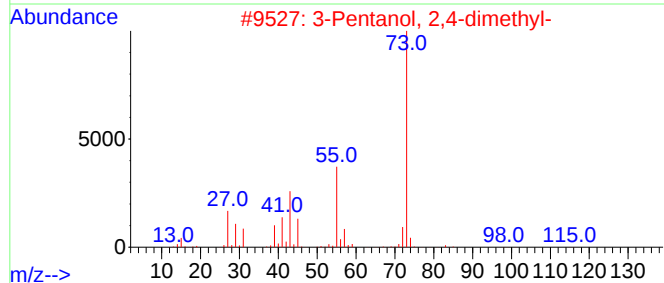
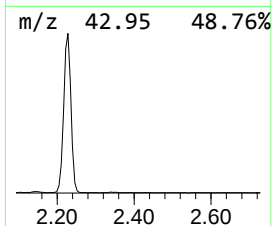
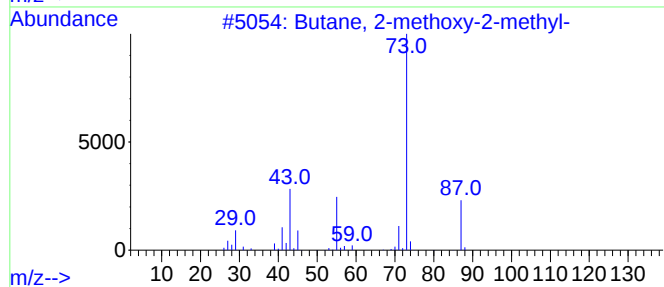
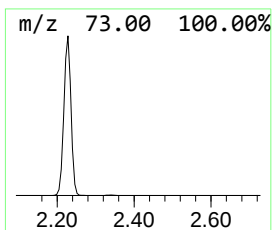
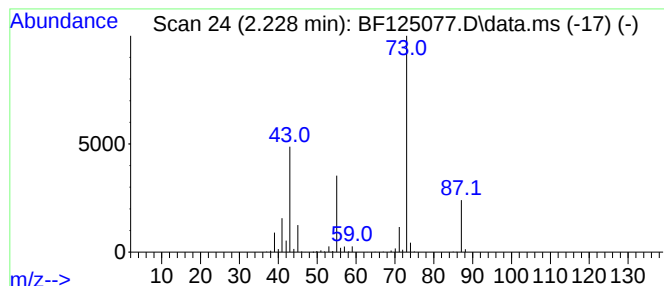
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.228	38.79 ng	1926590	1,4-Dichlorobenzene-d4	6.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	28



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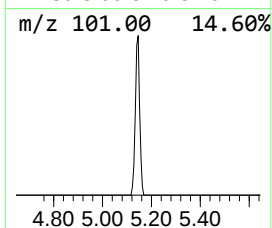
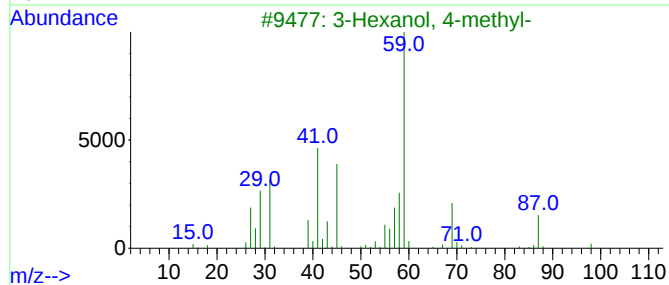
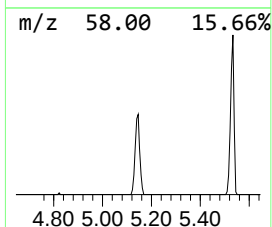
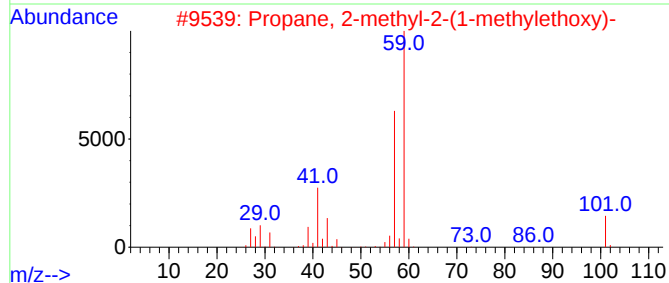
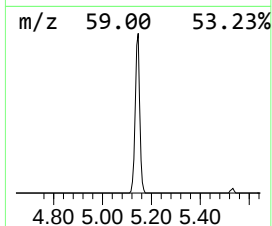
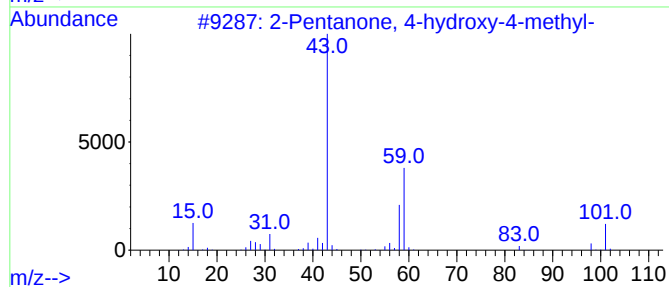
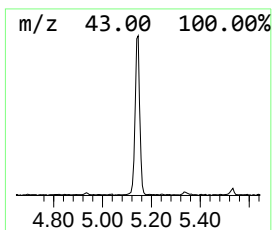
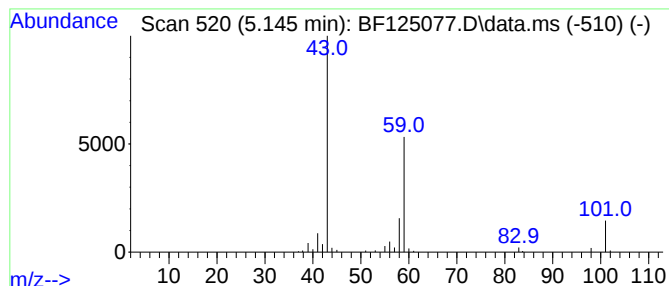
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.145	5.60 ng	278317	1,4-Dichlorobenzene-d4	6.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36		
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25		



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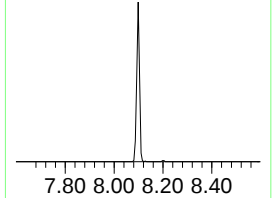
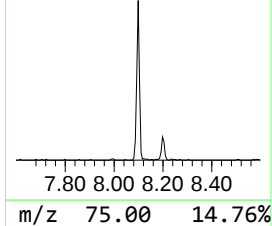
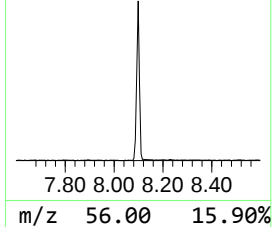
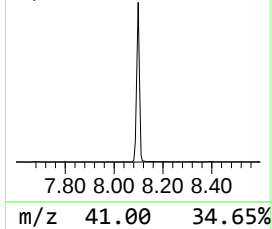
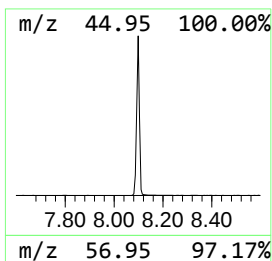
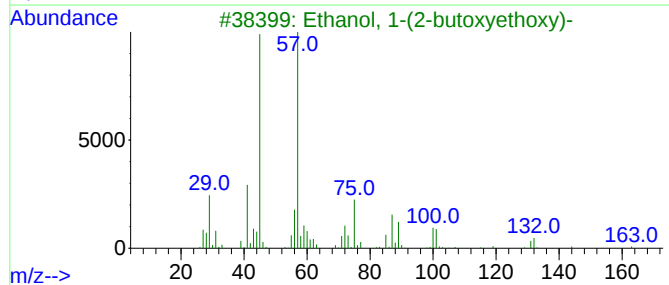
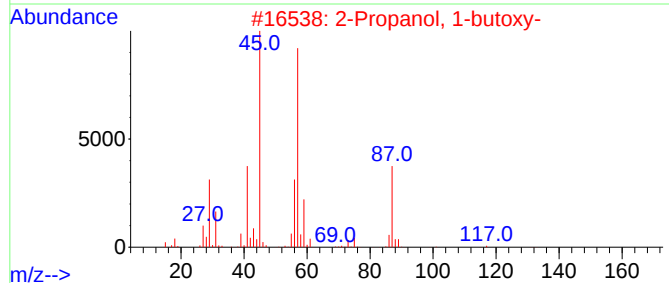
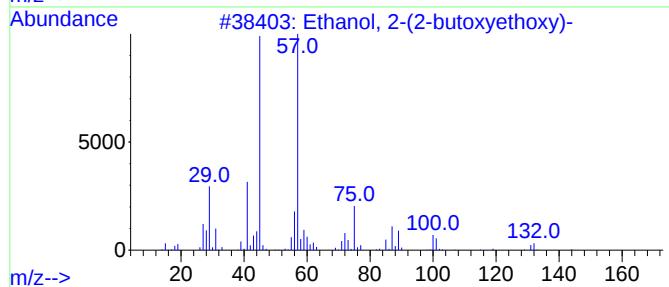
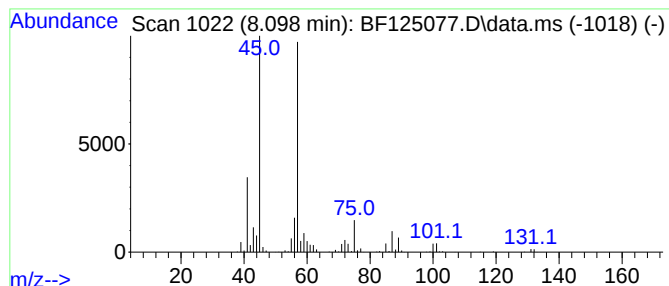
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.098	22.83 ng	1479240	Naphthalene-d8	8.204

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
2			2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	59
3			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	52
4			1-Methoxy-3-methyl-3-butene	100	C6H12O	034752-58-4	47
5			Butyl lactate	146	C7H14O3	000138-22-7	47



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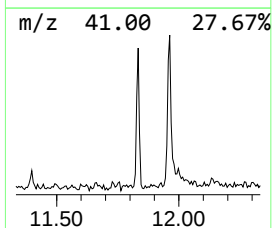
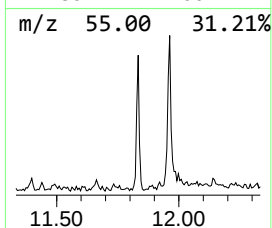
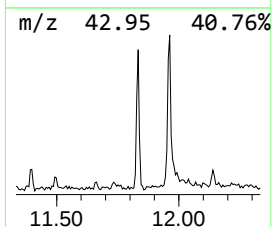
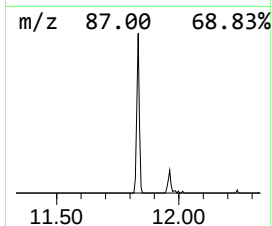
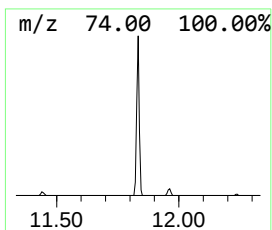
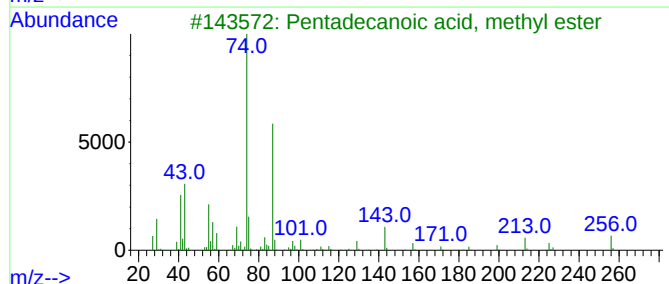
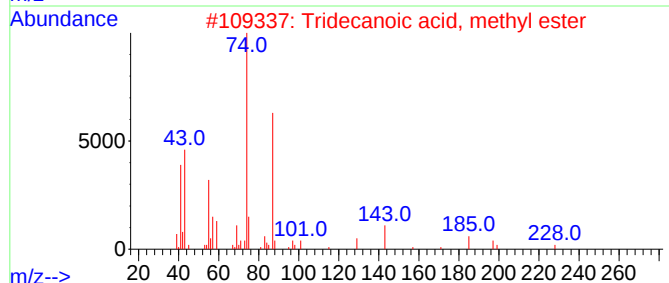
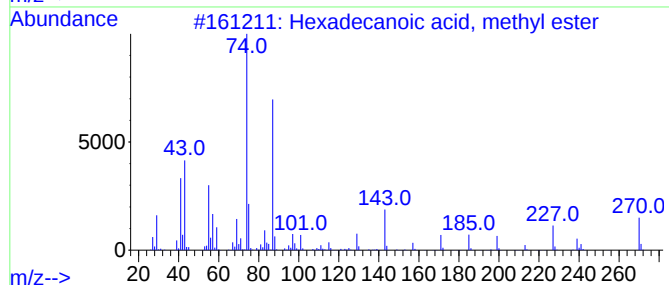
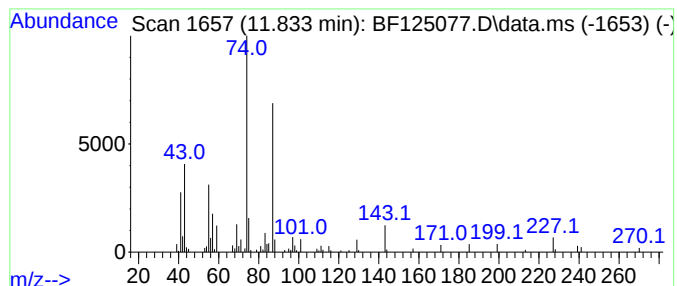
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Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.833	2.26 ng	155668	Phenanthrene-d10	11.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	97
2			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
3			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
4			Methyl tetradecanoate	242	C15H30O2	000124-10-7	90
5			Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	86



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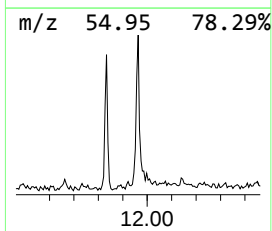
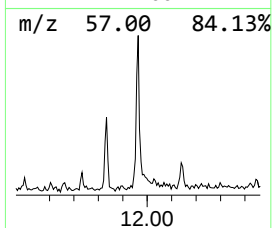
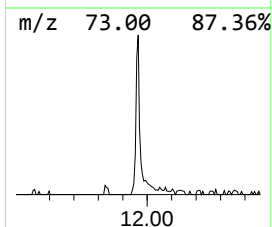
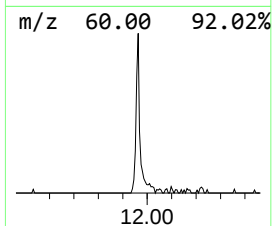
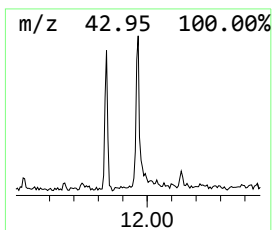
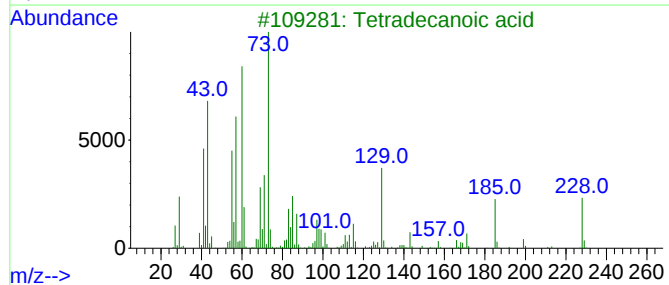
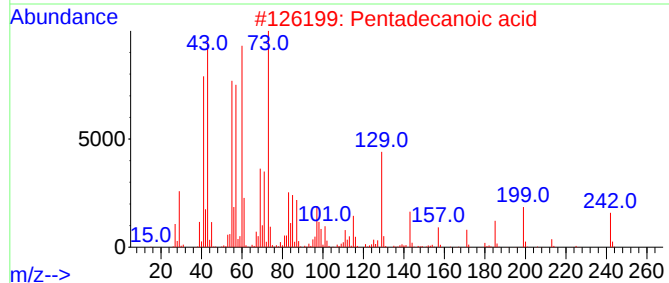
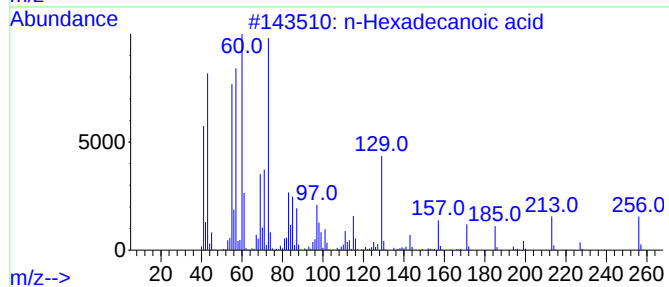
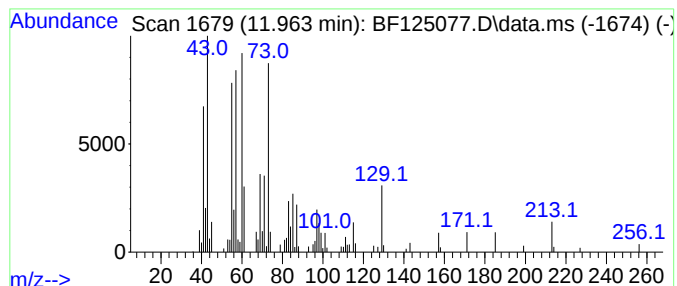
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.963	2.98 ng	205023	Phenanthrene-d10		11.445	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	91
2	Pentadecanoic acid		242	C15H30O2	001002-84-2	74
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	64
4	Tridecanoic acid		214	C13H26O2	000638-53-9	62
5	Dodecanoic acid		200	C12H24O2	000143-07-7	59



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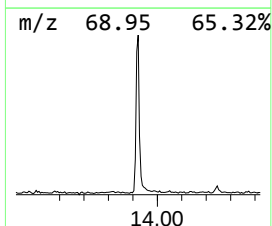
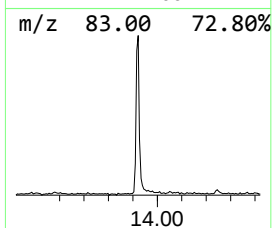
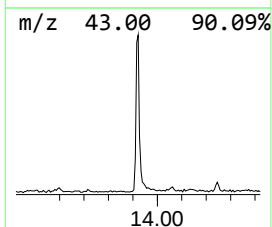
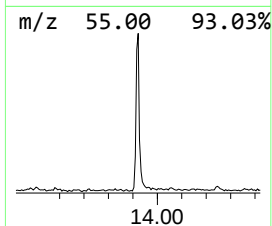
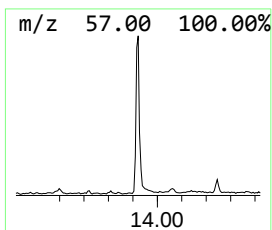
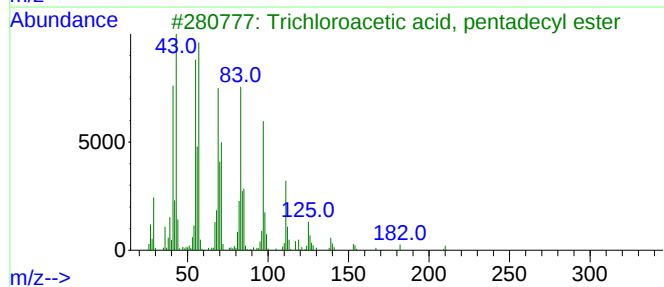
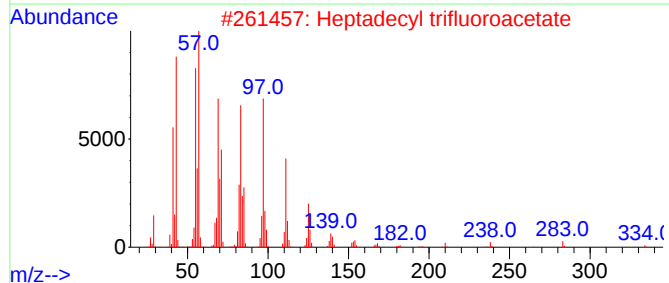
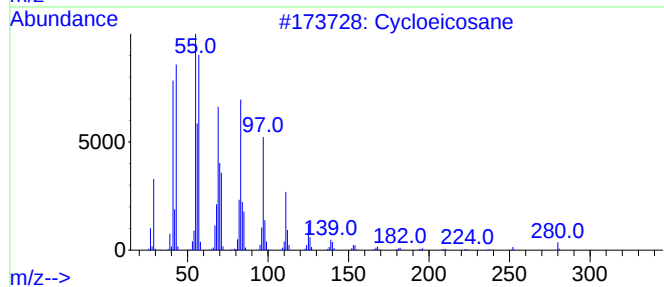
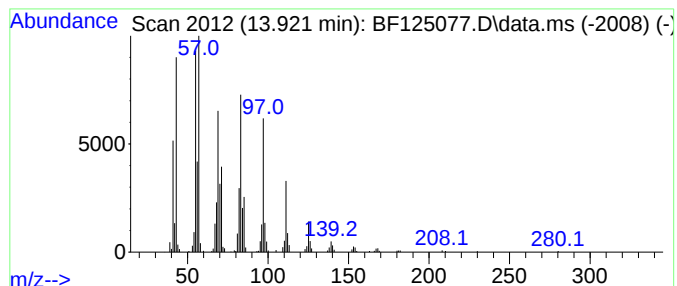
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cycloeicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.921	12.42 ng	682001	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cycloeicosane	280	C20H40	000296-56-0	95
2			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
3			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
4			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
5			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081721\
Data File : BF125077.D
Acq On : 17 Aug 2021 20:01
Operator : JU/CG
Sample : M3428-17
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-06-COMP

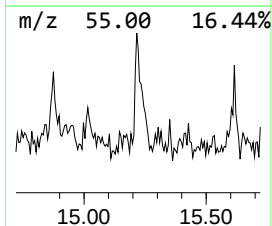
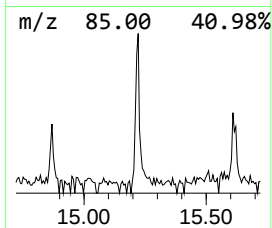
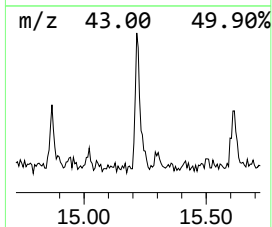
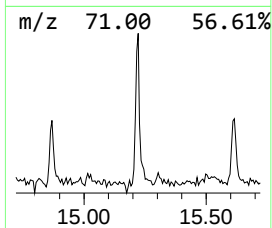
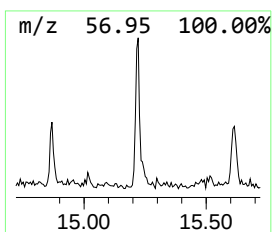
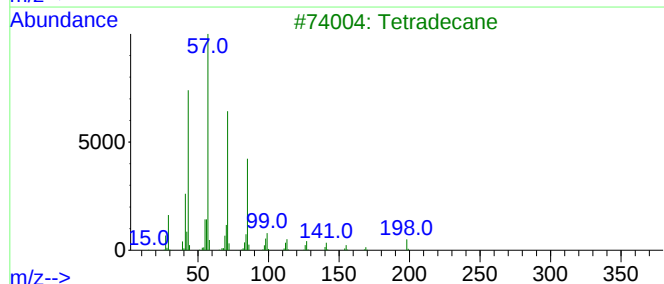
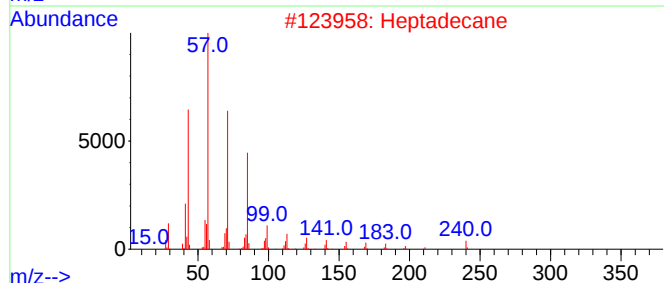
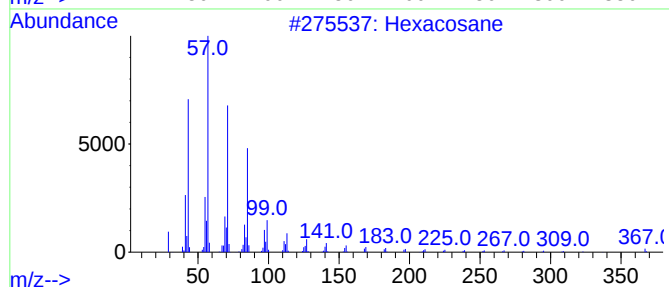
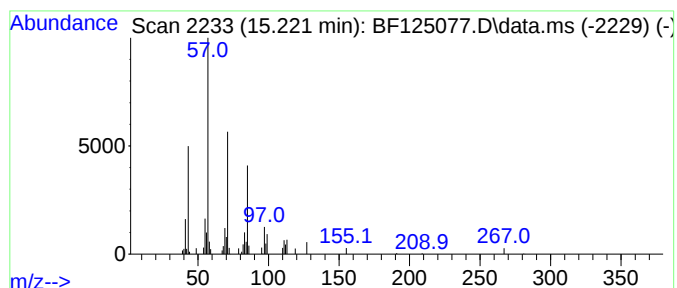
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.221	2.63 ng	92313	Perylene-d12	15.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	87
2			Heptadecane	240	C17H36	000629-78-7	86
3			Tetradecane	198	C14H30	000629-59-4	86
4			Octadecane	254	C18H38	000593-45-3	80
5			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081721\
Data File : BF125077.D
Acq On : 17 Aug 2021 20:01
Operator : JU/CG
Sample : M3428-17
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-06-COMP

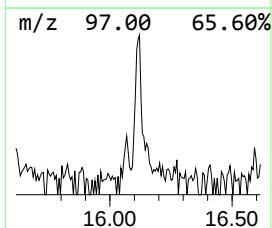
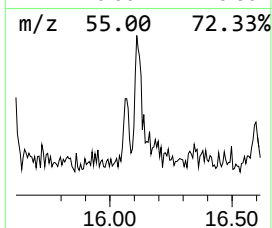
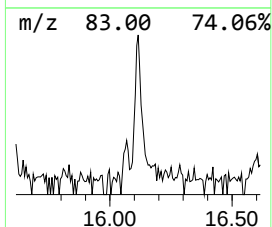
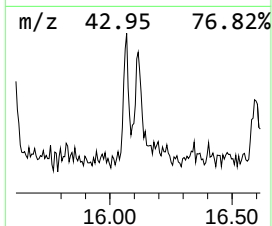
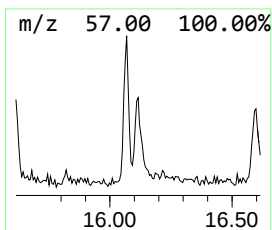
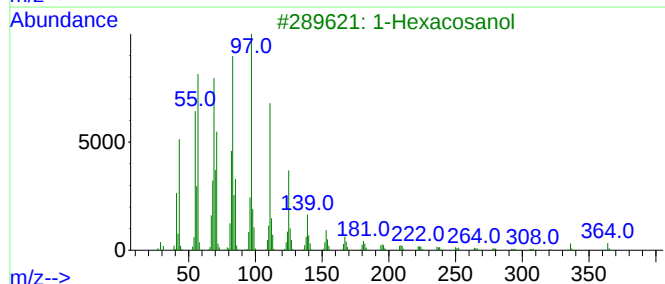
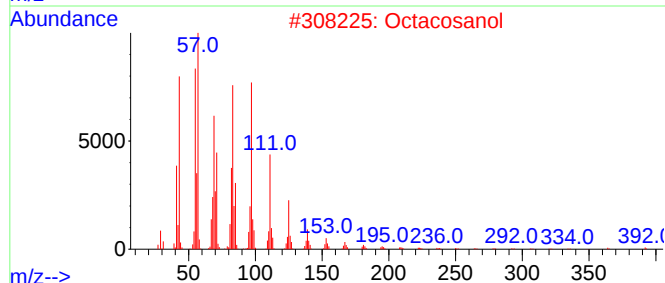
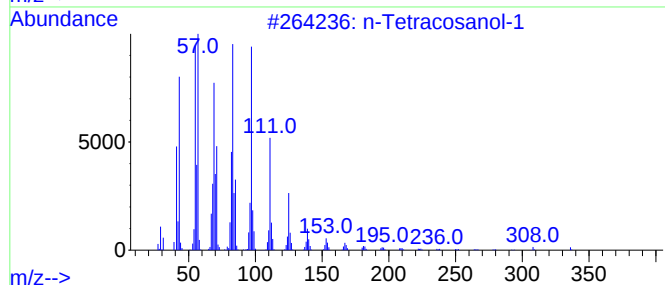
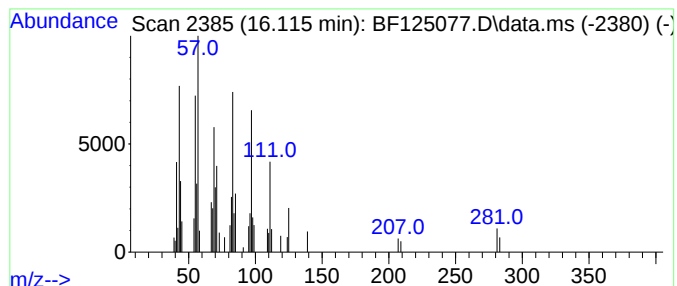
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Tetracosanol-1 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.115	2.44 ng	85639	Perylene-d12	15.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1			354	C24H50O	000506-51-4	93
2	Octacosanol			410	C28H58O	000557-61-9	90
3	1-Hexacosanol			382	C26H54O	000506-52-5	90
4	Heptadecyl trifluoroacetate			352	C19H35F3O2	1010351-87-0	90
5	1-Hexacosene			364	C26H52	018835-33-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081721\
Data File : BF125077.D
Acq On : 17 Aug 2021 20:01
Operator : JU/CG
Sample : M3428-17
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-06-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081721.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...	2.228	38.8	ng	1926590	1	6.922	993402	20.0
2-Pentanone, 4-...	5.145	5.6	ng	278317	1	6.922	993402	20.0
Ethanol, 2-(2-b...	8.098	22.8	ng	1479240	2	8.204	1295720	20.0
Hexadecanoic ac...	11.833	2.3	ng	155668	4	11.445	1377100	20.0
n-Hexadecanoic ...	11.963	3.0	ng	205023	4	11.445	1377100	20.0
Cycloeicosane	13.921	12.4	ng	682001	5	14.080	1098150	20.0
Hexacosane	15.221	2.6	ng	92313	6	15.574	702470	20.0
n-Tetracosanol-1	16.115	2.4	ng	85639	6	15.574	702470	20.0