

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083021\
 Data File : BF125268.D
 Acq On : 30 Aug 2021 18:15
 Operator : JU/CG
 Sample : M3561-11
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DUPLICATE-082521

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-BF081821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125268.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	8	14	27	rVB	3172555	4227850	75.34%	11.247%
2	5.528	581	585	588	rBV	2520696	2254153	40.17%	5.996%
3	6.534	752	756	766	rBV	1669187	1417027	25.25%	3.769%
4	6.910	817	820	824	rBV	1111332	981355	17.49%	2.611%
5	7.451	909	912	913	rBV	218229	183347	3.27%	0.488%
6	7.475	913	916	919	rVB	3147548	2990984	53.30%	7.956%
7	8.098	1013	1022	1035	rBV	389459	660531	11.77%	1.757%
8	8.198	1035	1039	1042	rBV	1491643	1283757	22.88%	3.415%
9	8.557	1093	1100	1102	rBV3	44996	65519	1.17%	0.174%
10	8.892	1154	1157	1159	rBV2	51023	63804	1.14%	0.170%
11	9.222	1210	1213	1215	rBV4	47346	70315	1.25%	0.187%
12	9.269	1217	1221	1224	rBV	5709854	5149879	91.77%	13.699%
13	9.504	1258	1261	1263	rBV2	119046	139819	2.49%	0.372%
14	9.533	1263	1266	1268	rVV2	114383	106015	1.89%	0.282%
15	9.616	1276	1280	1285	rBV5	111190	254502	4.54%	0.677%
16	9.704	1293	1295	1300	rBV4	73683	113862	2.03%	0.303%
17	9.951	1334	1337	1343	rVB	1815272	1460101	26.02%	3.884%
18	10.333	1398	1402	1405	rBV	1890627	1572714	28.02%	4.184%
19	10.469	1423	1425	1430	rVB	196777	209894	3.74%	0.558%
20	10.516	1430	1433	1436	rBV3	126026	190641	3.40%	0.507%
21	10.745	1468	1472	1475	rBV	3983354	3765985	67.11%	10.018%
22	11.439	1587	1590	1593	rBV	1847340	1470484	26.20%	3.912%
23	11.551	1607	1609	1614	rVB2	163596	130028	2.32%	0.346%
24	11.963	1676	1679	1683	rBV	406927	347108	6.19%	0.923%
25	12.745	1809	1812	1817	rVB	227740	214849	3.83%	0.572%
26	13.027	1855	1860	1863	rBV	6212022	5611923	100.00%	14.928%
27	13.927	2011	2013	2019	rVB3	97211	118307	2.11%	0.315%
28	14.080	2035	2039	2043	rVB	1281284	1076055	19.17%	2.862%
29	15.580	2289	2294	2310	rVB	991573	1461709	26.05%	3.888%

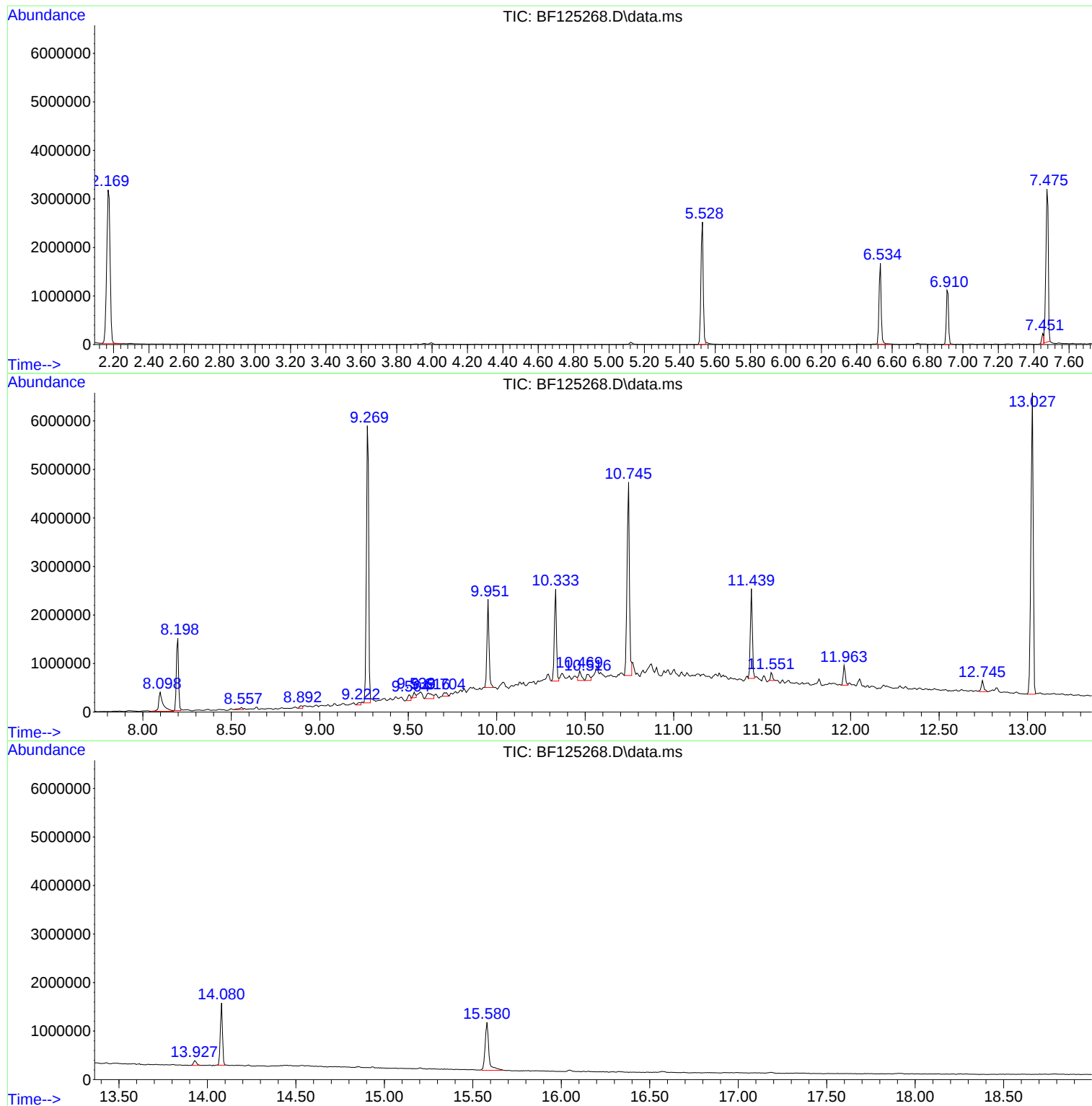
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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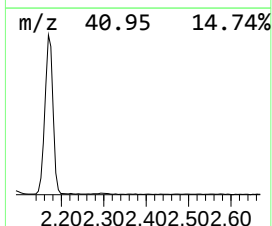
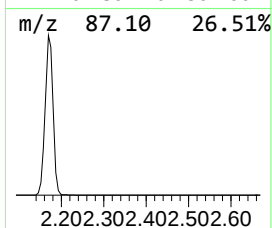
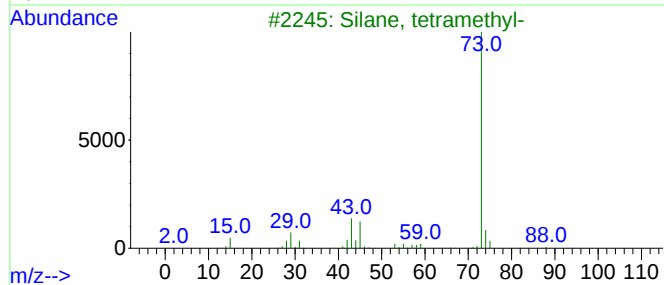
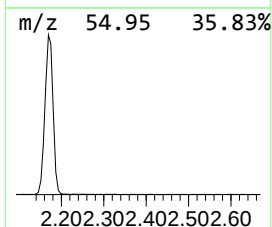
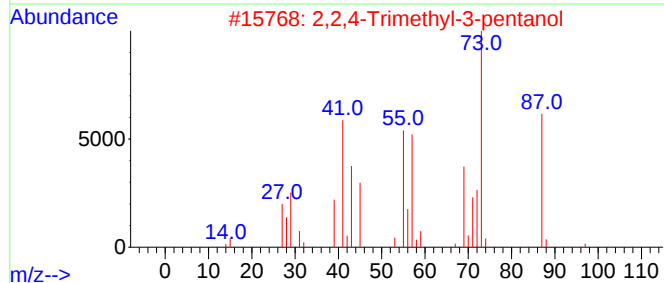
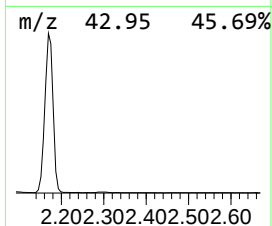
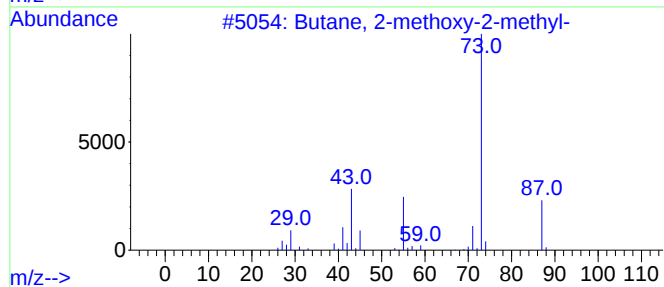
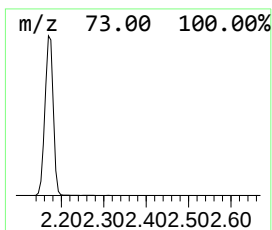
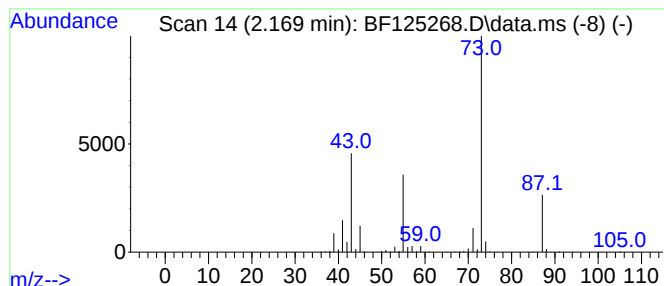
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.169	86.16 ng	4227850	1,4-Dichlorobenzene-d4	6.916

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			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	23
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



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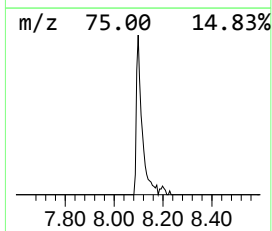
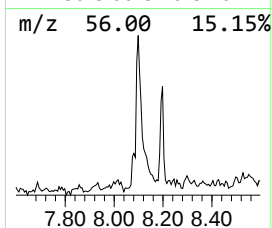
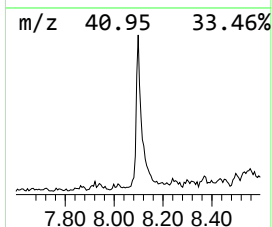
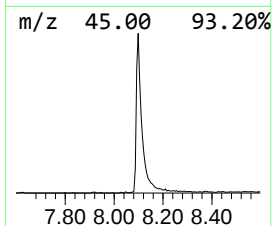
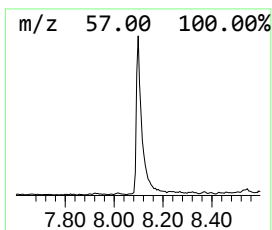
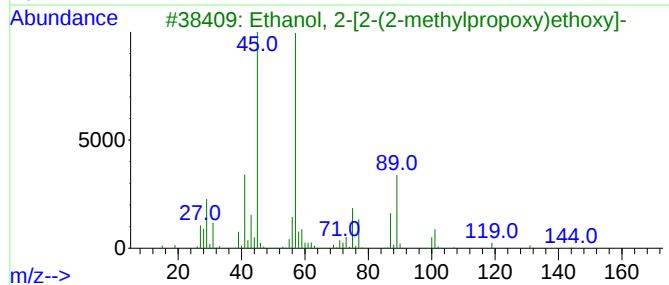
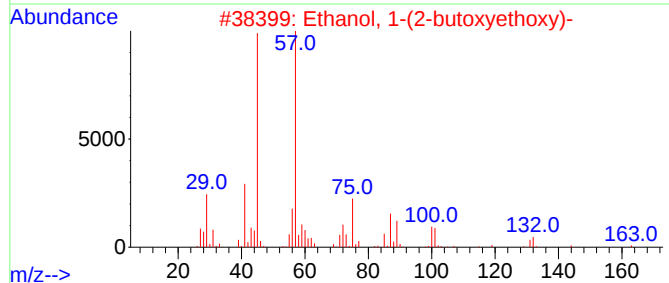
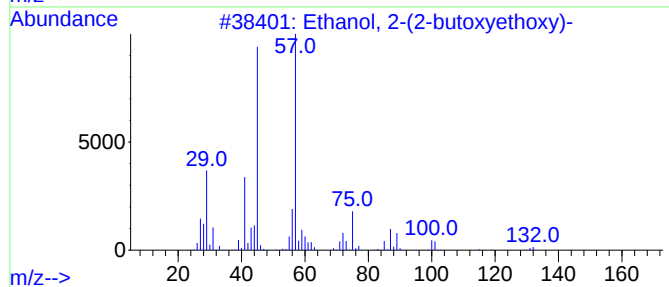
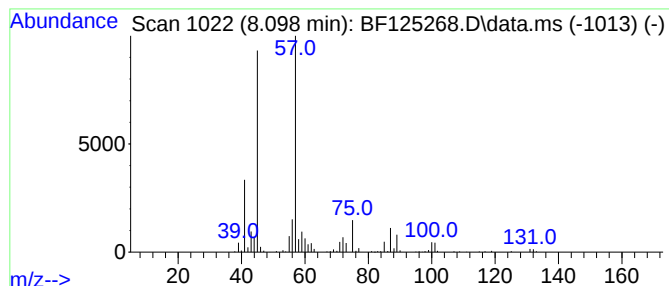
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.098	10.29 ng	660531	Naphthalene-d8	8.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
4			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
5			Tetraethylene glycol	194	C8H18O5	000112-60-7	50



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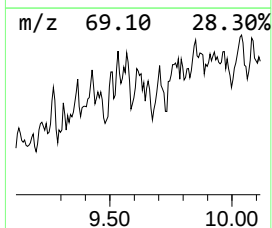
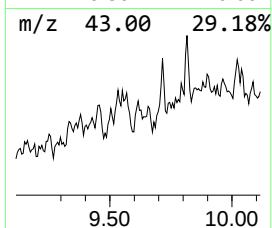
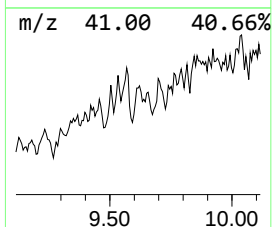
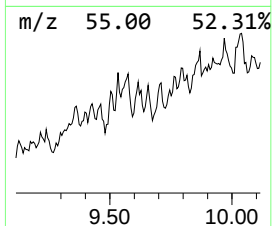
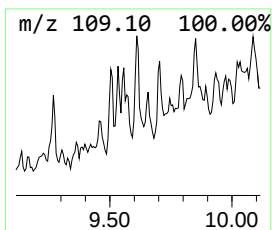
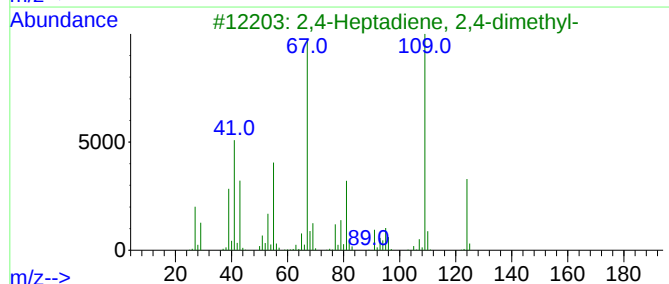
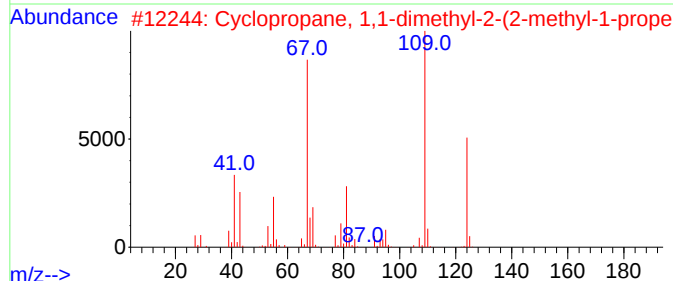
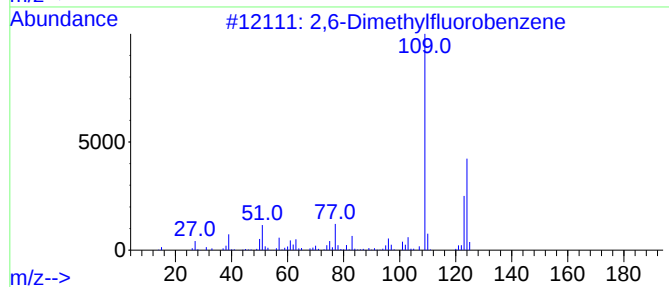
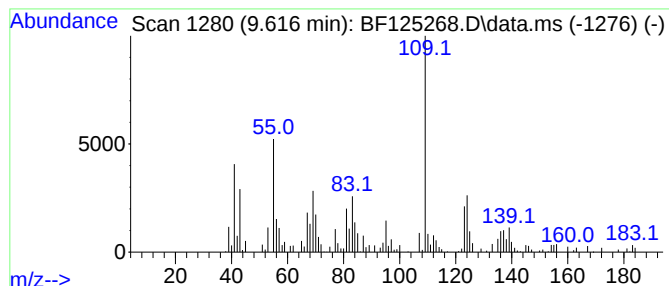
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2,6-Dimethylfluorobenzene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.616	3.49 ng	254502	Acenaphthene-d10	9.951

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,6-Dimethylfluorobenzene	124	C8H9F	000443-88-9	50
2			Cyclopropane, 1,1-dimethyl-2-(2-...	124	C9H16	033422-32-1	49
3			2,4-Heptadiene, 2,4-dimethyl-	124	C9H16	074421-05-9	49
4			2-Acetyl-5-methylfuran	124	C7H8O2	001193-79-9	46
5			2,5-Furandione, dihydro-3-(2-met...	154	C8H10O3	018908-20-8	46



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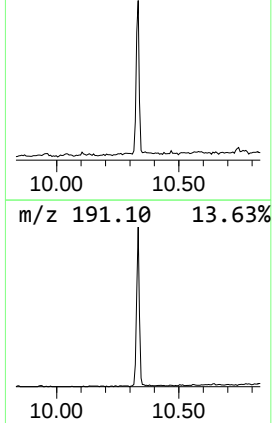
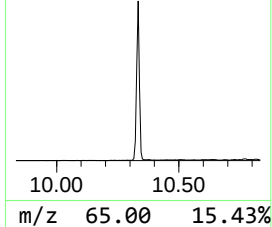
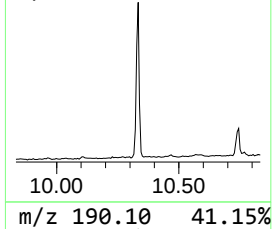
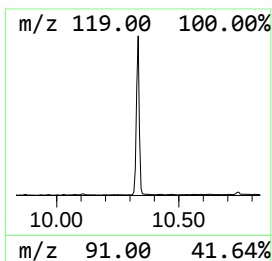
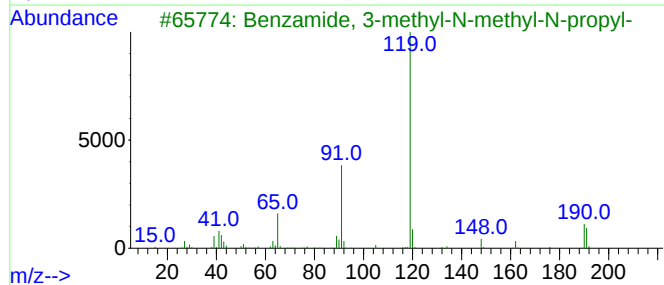
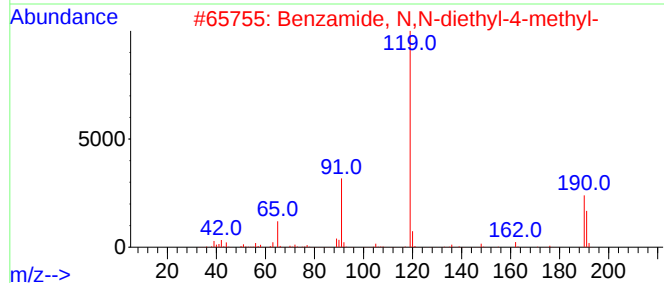
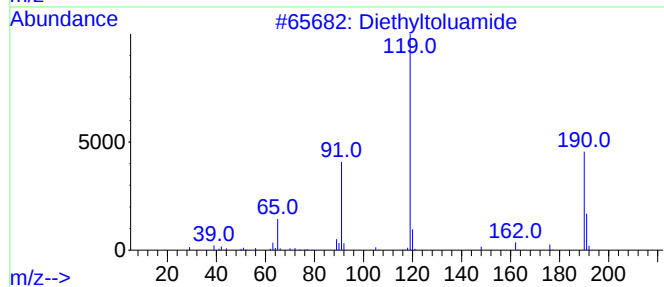
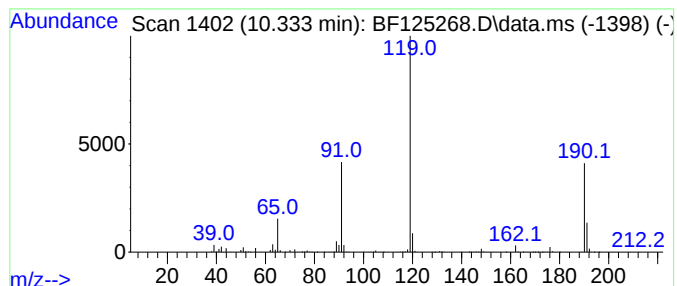
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Diethyltoluamide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.333	21.54 ng	1572710	Acenaphthene-d10	9.951

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethyltoluamide	191	C12H17NO	000134-62-3	97
2			Benzamide, N,N-diethyl-4-methyl-	191	C12H17NO	002728-05-4	81
3			Benzamide, 3-methyl-N-methyl-N-p...	191	C12H17NO	1000421-46-2	81
4			Benzamide, 4-methyl-N-butyl-	191	C12H17NO	1000407-46-6	76
5			Benzamide, 3-methyl-N-butyl-	191	C12H17NO	1000407-41-1	76



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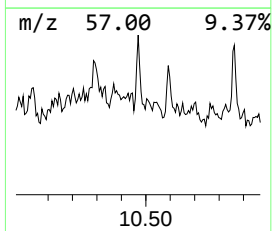
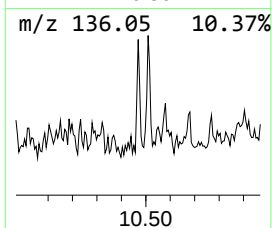
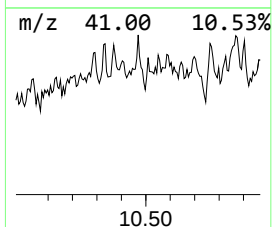
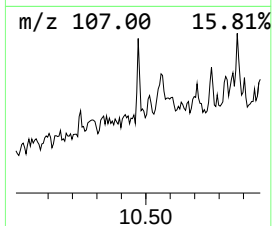
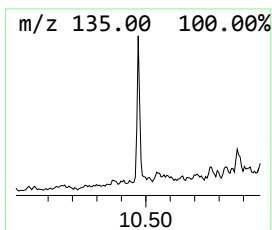
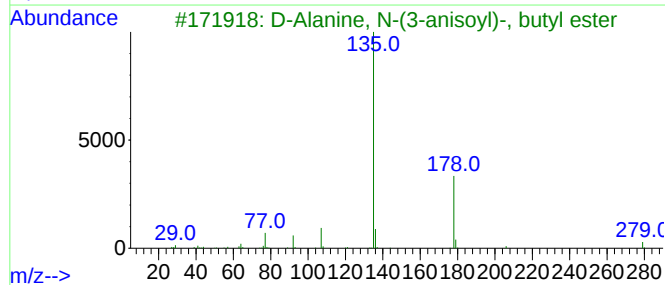
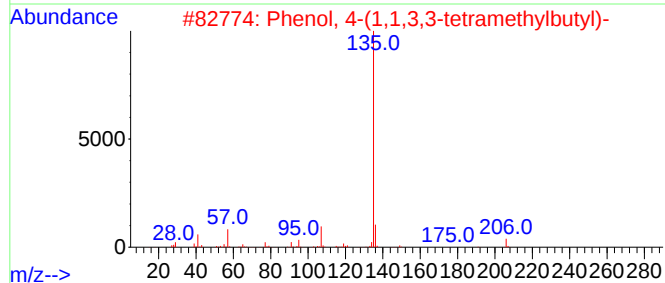
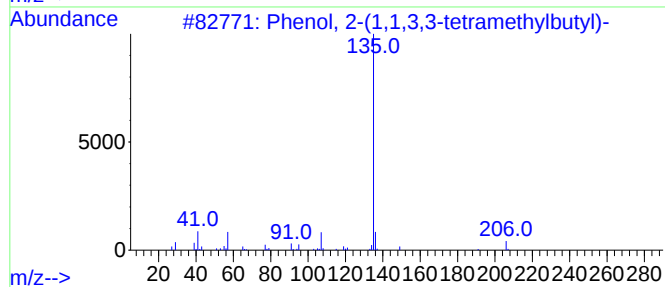
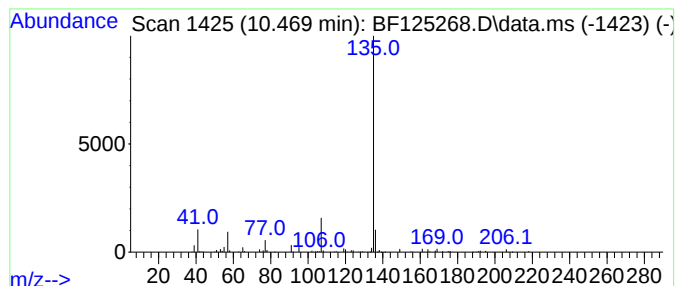
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Peak Number 5 Phenol, 2-(1,1,3,3-tetramet... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.469	2.88 ng	209894	Acenaphthene-d10	9.951

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2-(1,1,3,3-tetramethylbu...	206	C14H22O	003884-95-5	72
2			Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	72
3			D-Alanine, N-(3-anisoyl)-, butyl...	279	C15H21NO4	1000354-04-3	64
4			4-tert-Butylphenyl acetate	192	C12H16O2	003056-64-2	64
5			4-(1,1-Dimethylpropyl)phenyl ace...	206	C13H18O2	1000373-45-3	64



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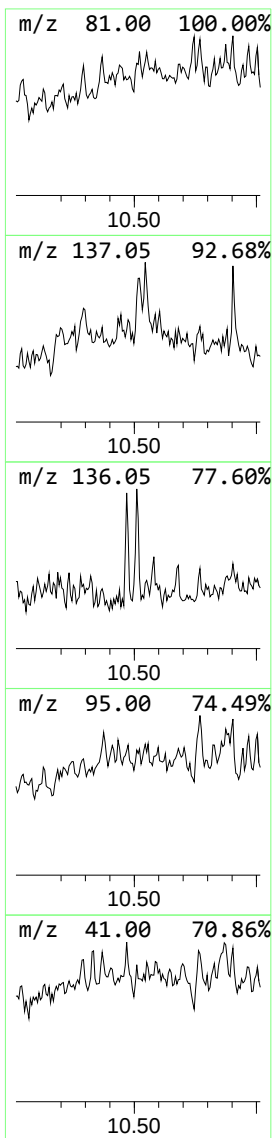
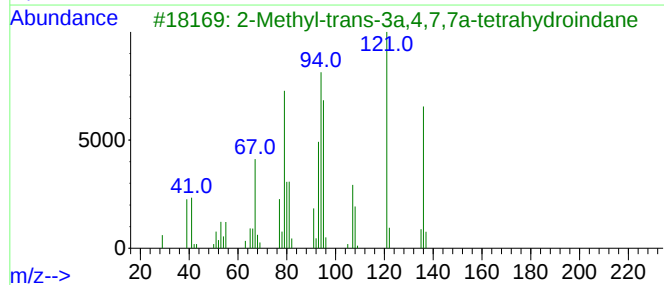
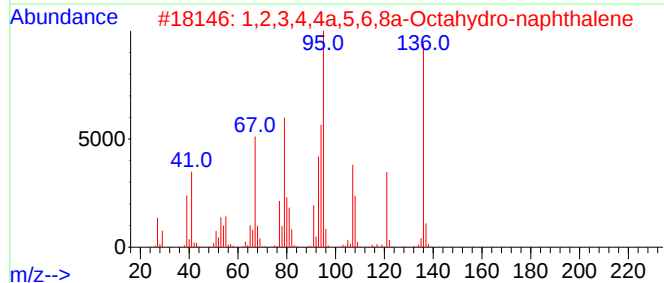
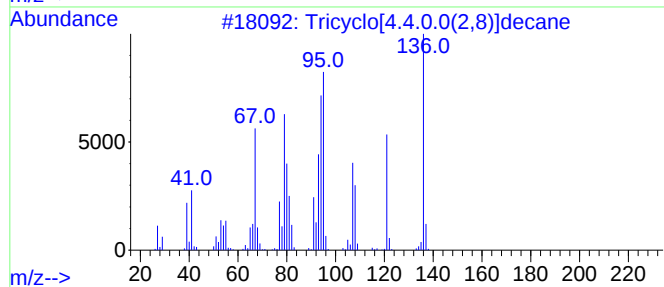
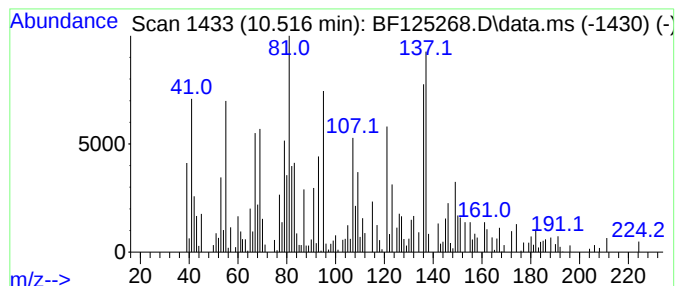
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown10.516 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.516	2.61 ng	190641	Acenaphthene-d10	9.951

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tricyclo[4.4.0.0(2,8)]decane	136	C10H16	049700-59-6	42
2			1,2,3,4,4a,5,6,8a-Octahydro-naph...	136	C10H16	031244-58-3	38
3			2-Methyl-trans-3a,4,7,7a-tetrahy...	136	C10H16	1000145-84-2	30
4			4-(2-Furyl)-2,4-dioxobutanoic acid	182	C8H6O5	1010484-30-9	30
5			2,5-Dimethylanisole	136	C9H12O	001706-11-2	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083021\
Data File : BF125268.D
Acq On : 30 Aug 2021 18:15
Operator : JU/CG
Sample : M3561-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUPLICATE-082521

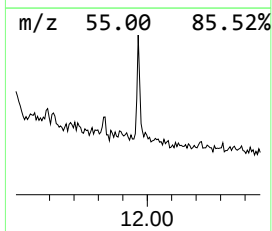
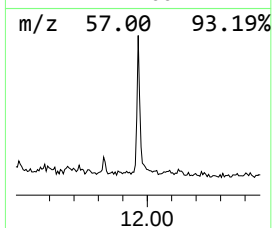
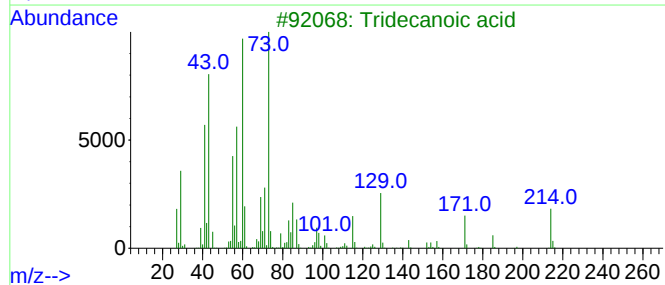
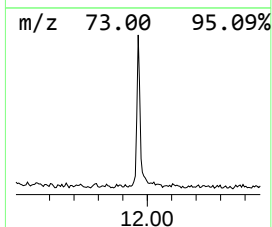
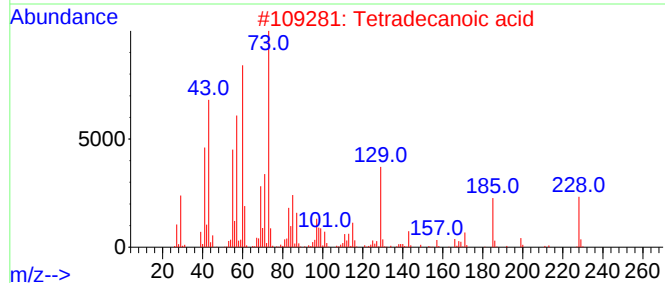
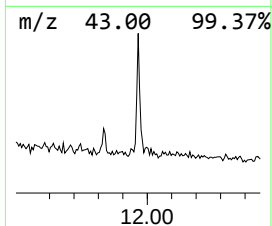
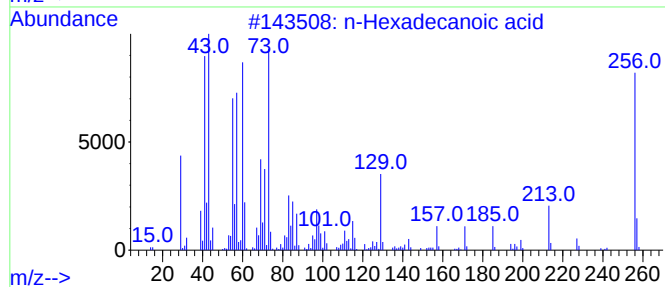
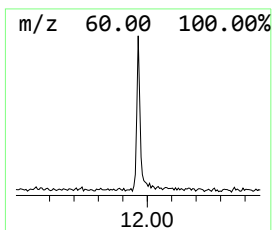
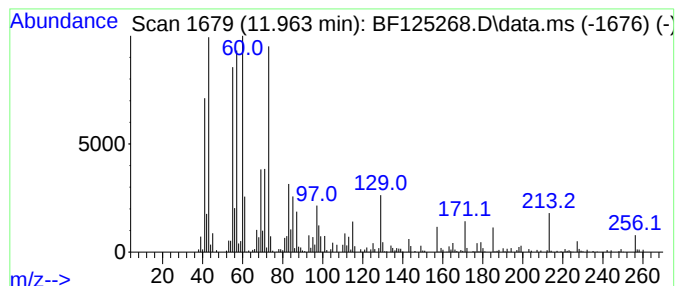
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.963	4.72 ng	347108	Phenanthrene-d10	11.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3			Tridecanoic acid	214	C13H26O2	000638-53-9	90
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083021\
Data File : BF125268.D
Acq On : 30 Aug 2021 18:15
Operator : JU/CG
Sample : M3561-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUPLICATE-082521

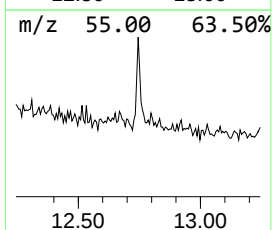
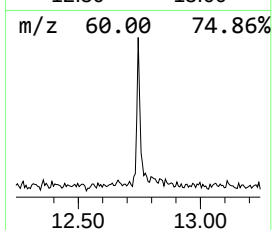
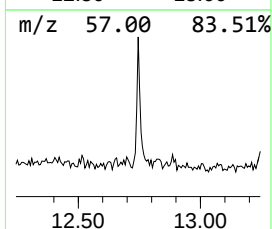
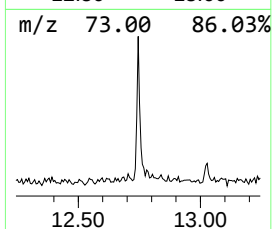
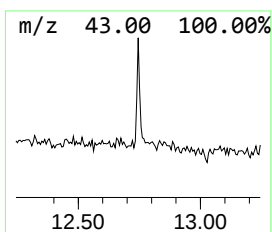
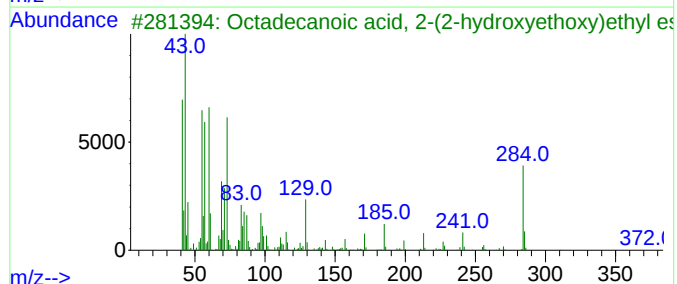
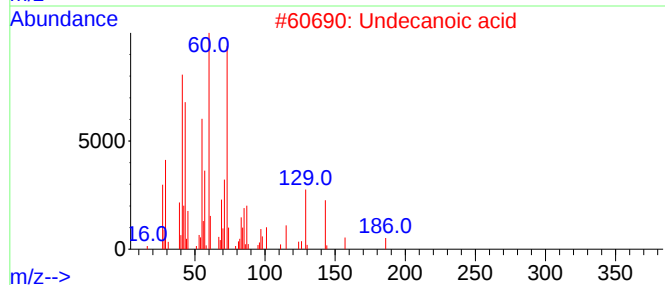
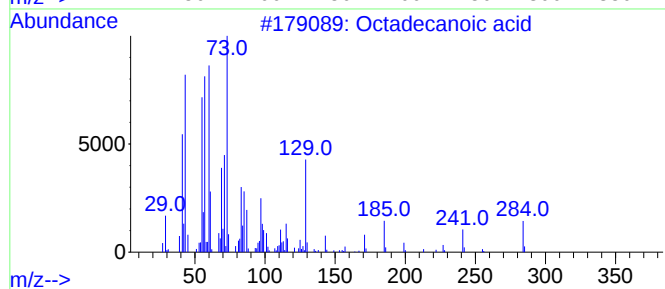
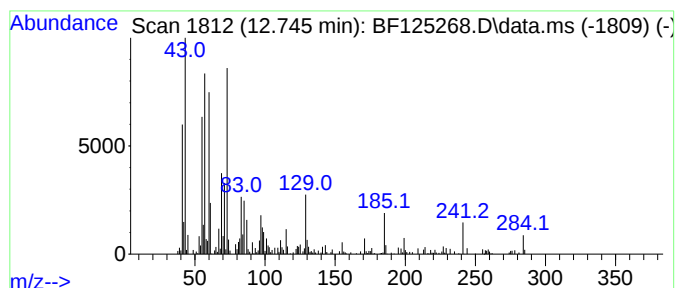
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.745	2.92 ng	214849	Phenanthrene-d10	11.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Undecanoic acid	186	C11H22O2	000112-37-8	86
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5			Tridecanoic acid	214	C13H26O2	000638-53-9	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083021\
Data File : BF125268.D
Acq On : 30 Aug 2021 18:15
Operator : JU/CG
Sample : M3561-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
DUPLICATE-082521

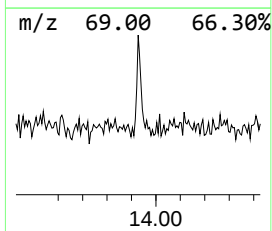
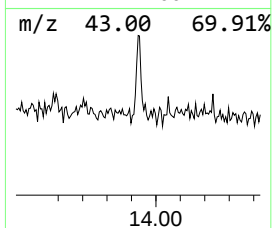
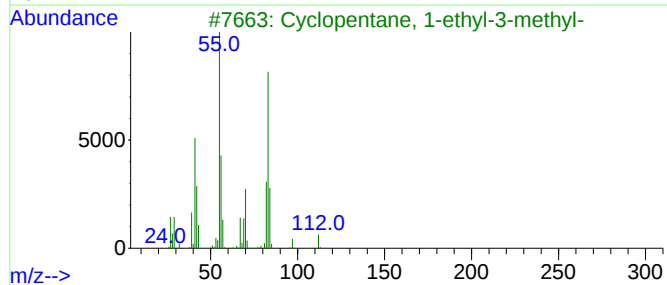
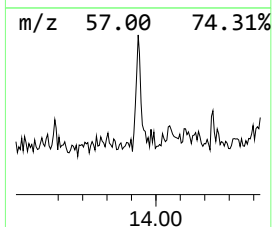
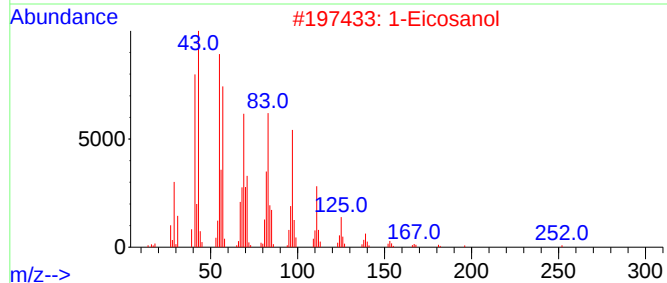
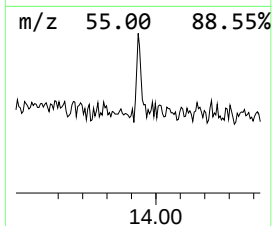
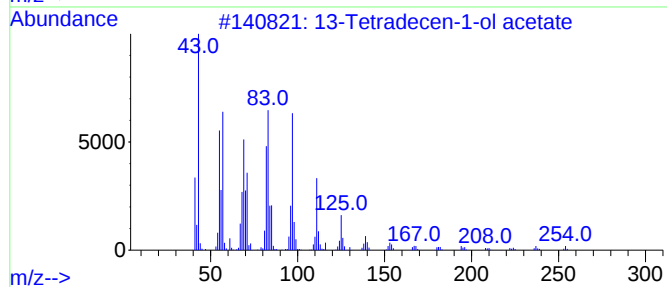
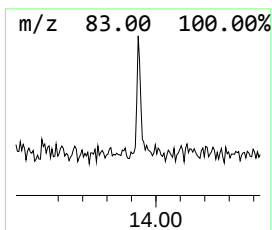
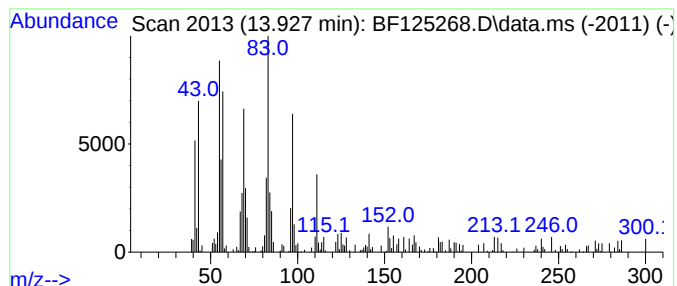
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 13-Tetradecen-1-ol acetate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.927	2.20 ng	118307	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	83
2			1-Eicosanol	298	C20H42O	000629-96-9	62
3			Cyclopentane, 1-ethyl-3-methyl-	112	C8H16	003726-47-4	60
4			1-Nonadecene	266	C19H38	018435-45-5	58
5			cis-1-Chloro-9-octadecene	286	C18H35Cl	016507-61-2	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083021\
Data File : BF125268.D
Acq On : 30 Aug 2021 18:15
Operator : JU/CG
Sample : M3561-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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...	2.169	86.2	ng	4227850	1	6.916	981355	20.0
Ethanol, 2-(2-b...	8.098	10.3	ng	660531	2	8.198	1283760	20.0
2,6-Dimethylflu...	9.616	3.5	ng	254502	3	9.951	1460100	20.0
Diethyltoluamide	10.333	21.5	ng	1572710	3	9.951	1460100	20.0
Phenol, 2-(1,1,...	10.469	2.9	ng	209894	3	9.951	1460100	20.0
unknown10.516	10.516	2.6	ng	190641	3	9.951	1460100	20.0
n-Hexadecanoic ...	11.963	4.7	ng	347108	4	11.439	1470480	20.0
Octadecanoic acid	12.745	2.9	ng	214849	4	11.439	1470480	20.0
13-Tetradecen-1...	13.927	2.2	ng	118307	5	14.080	1076060	20.0