

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083121\
 Data File : BF125287.D
 Acq On : 31 Aug 2021 14:21
 Operator : JU/CG
 Sample : M3561-05
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 OUII-E

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: BF125287.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	11	17	30	rVB	3091109	4128981	58.18%	10.301%
2	5.534	582	586	598	rBV	2458016	2220979	31.30%	5.541%
3	6.539	753	757	764	rBV	1504559	1353056	19.07%	3.375%
4	6.910	817	820	824	rBV	1223332	1055017	14.87%	2.632%
5	7.481	911	917	920	rBV	3183957	3231255	45.53%	8.061%
6	8.098	1018	1022	1035	rBV	567035	837027	11.79%	2.088%
7	8.198	1035	1039	1042	rVV	1632446	1380032	19.45%	3.443%
8	9.269	1217	1221	1231	rBV	5763645	5615496	79.13%	14.009%
9	9.345	1231	1234	1237	rVB2	75299	74819	1.05%	0.187%
10	9.657	1284	1287	1290	rVB2	189819	177889	2.51%	0.444%
11	9.816	1311	1314	1316	rBV2	79802	77754	1.10%	0.194%
12	9.857	1319	1321	1324	rVB	147378	129691	1.83%	0.324%
13	9.951	1331	1337	1341	rBV	1912492	1674723	23.60%	4.178%
14	10.327	1397	1401	1403	rBV3	63777	81493	1.15%	0.203%
15	10.745	1467	1472	1475	rBV	4041534	3996149	56.31%	9.969%
16	10.857	1488	1491	1494	rVB	142845	117077	1.65%	0.292%
17	11.321	1567	1570	1572	rBV2	83384	71601	1.01%	0.179%
18	11.439	1586	1590	1593	rBV	2091788	1739113	24.51%	4.339%
19	11.821	1652	1655	1658	rVB	177233	139698	1.97%	0.349%
20	11.957	1673	1678	1688	rBV2	789933	867707	12.23%	2.165%
21	12.663	1796	1798	1807	rVB2	99047	145574	2.05%	0.363%
22	12.739	1808	1811	1819	rVV	290274	321520	4.53%	0.802%
23	13.027	1855	1860	1863	rBV	6752095	7096628	100.00%	17.704%
24	13.392	1918	1922	1928	rBV3	78950	151827	2.14%	0.379%
25	13.945	2012	2016	2027	rVB	216742	344438	4.85%	0.859%
26	14.080	2035	2039	2046	rVB	1722574	1579496	22.26%	3.940%
27	14.645	2131	2135	2140	rVB2	110095	171851	2.42%	0.429%
28	14.704	2142	2145	2150	rVB7	56443	80013	1.13%	0.200%
29	15.580	2289	2294	2301	rBV	930211	1224326	17.25%	3.054%

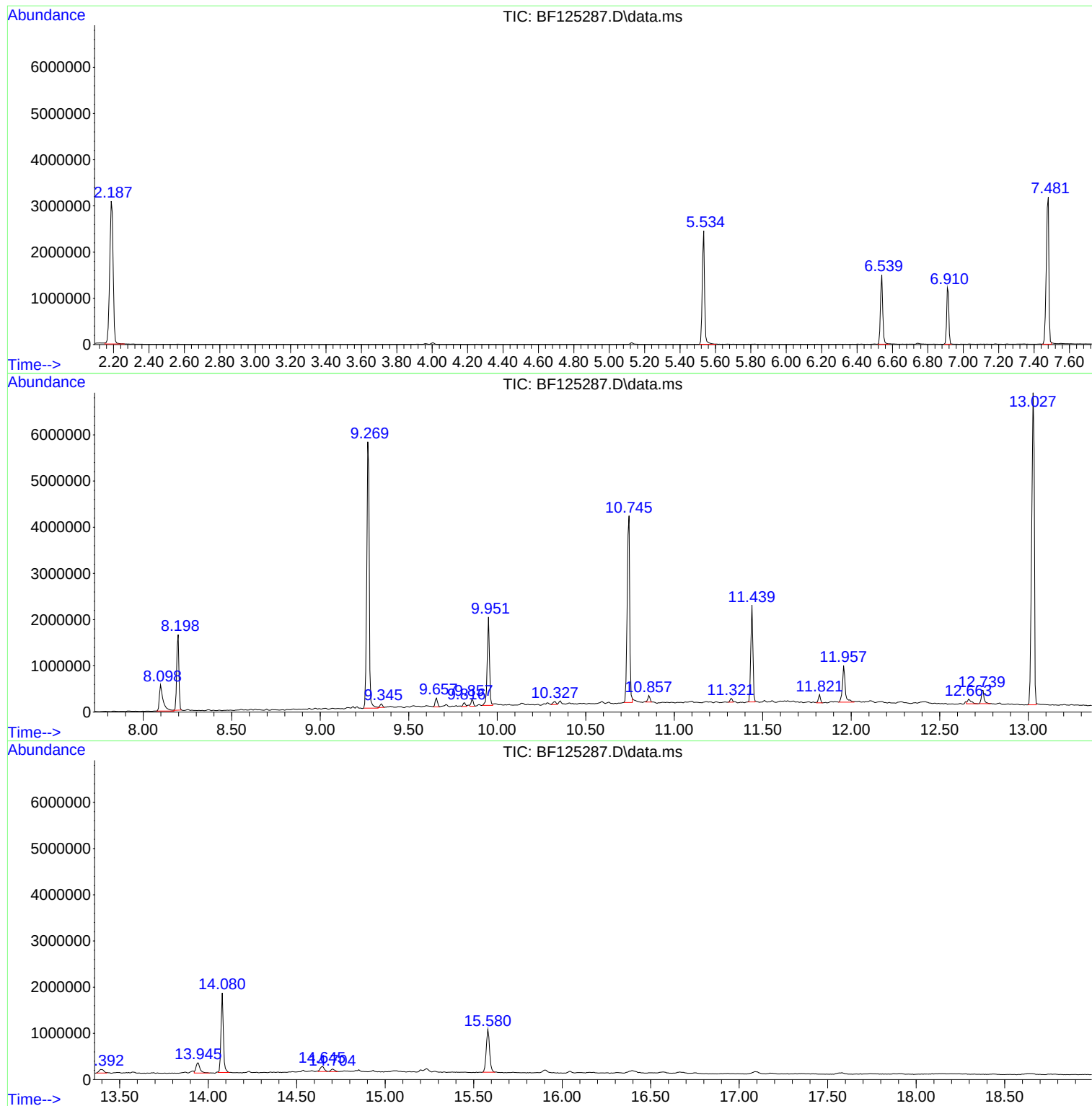
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Instrument :
BNA_F
ClientSampleId :
OUII-E

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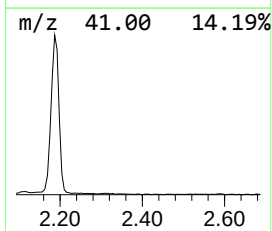
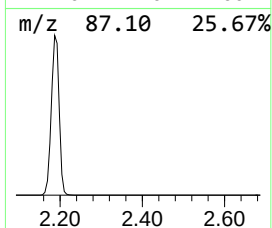
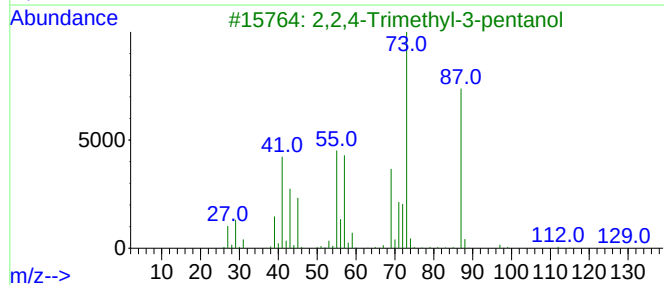
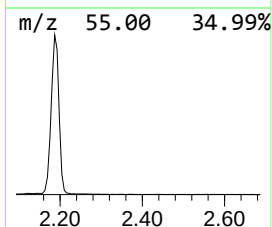
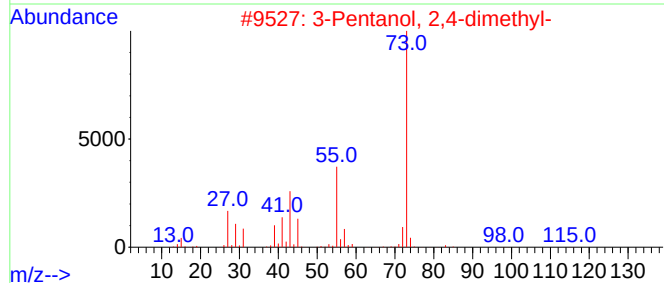
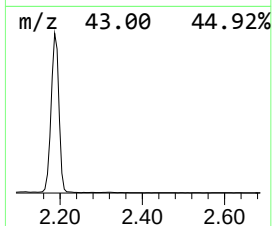
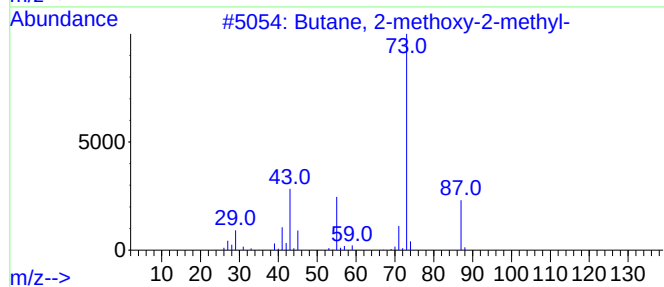
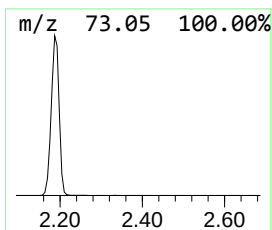
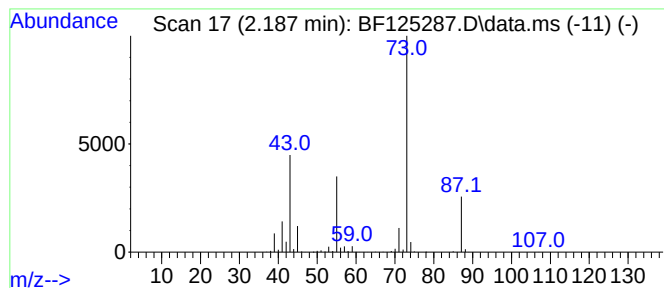
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.187	78.27 ng	4128980	1,4-Dichlorobenzene-d4	6.910

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			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23



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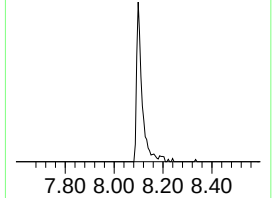
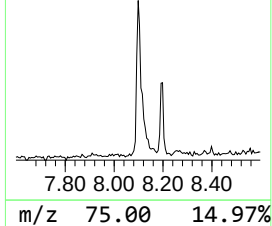
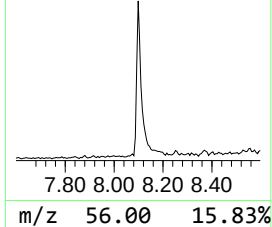
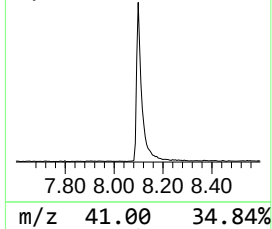
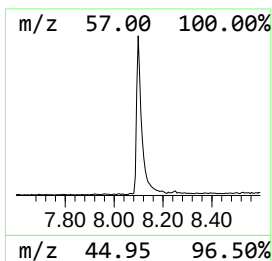
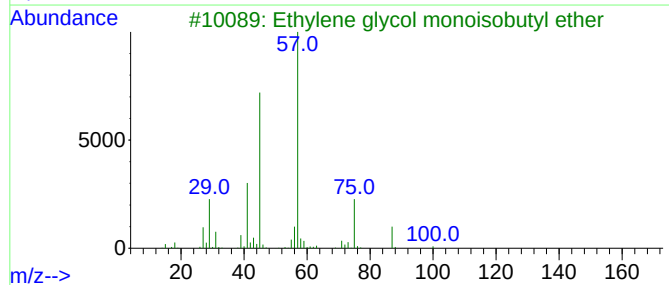
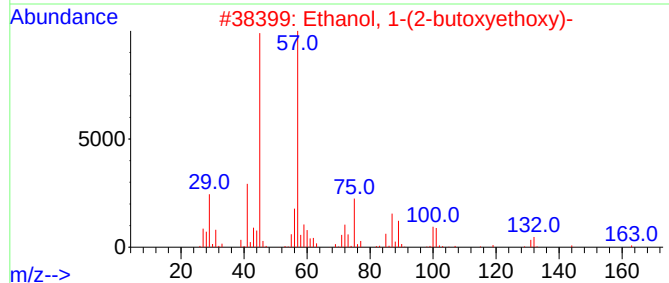
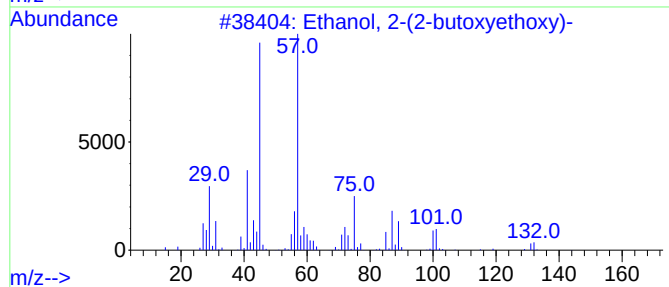
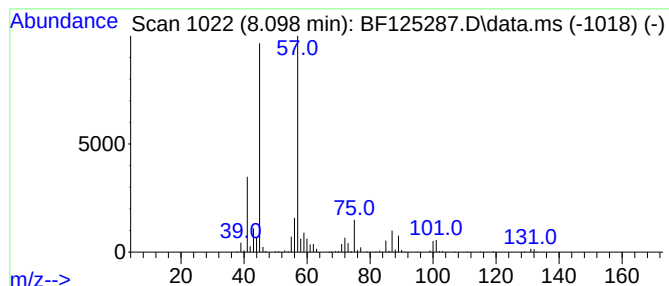
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.098	12.13 ng	837027	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			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
4			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	56
5			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53



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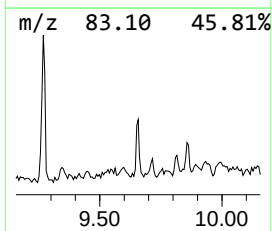
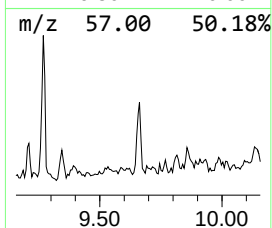
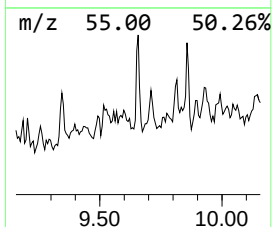
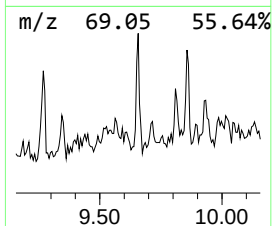
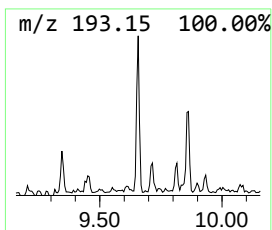
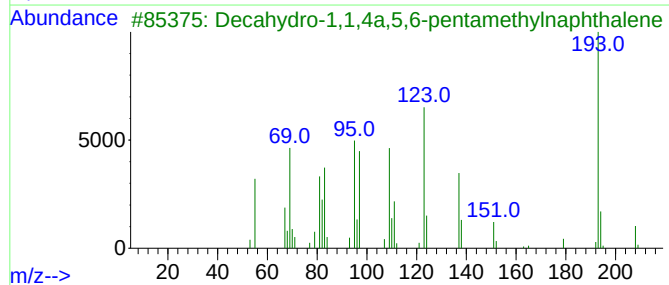
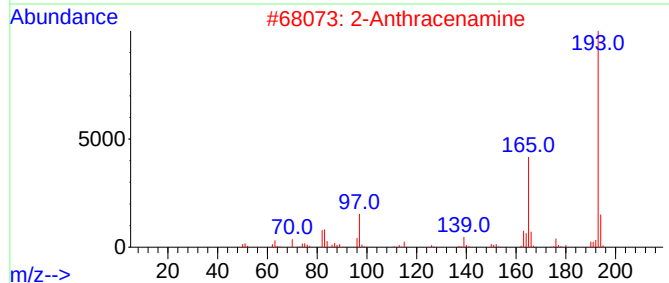
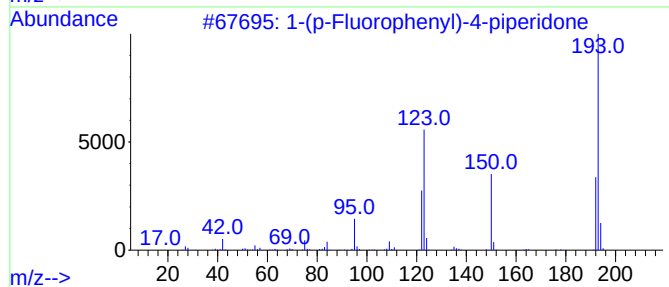
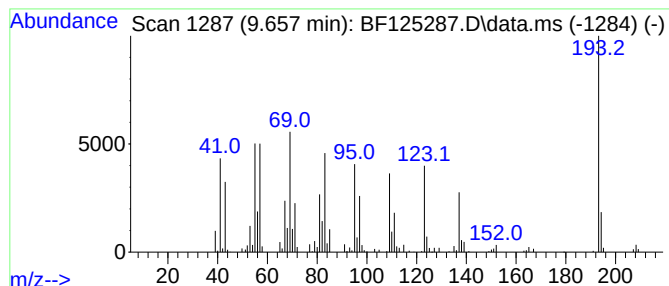
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Peak Number 3 unknown9.657 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.657	2.12 ng	177889	Acenaphthene-d10	9.951

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	43		
2	2-Anthracenamine	193	C14H11N	000613-13-8	25		
3	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	22		
4	9-Phenanthrenamine	193	C14H11N	000947-73-9	22		
5	11-Dodecen-2-one, 7,7-dimethyl-	210	C14H26O	035194-22-0	22		



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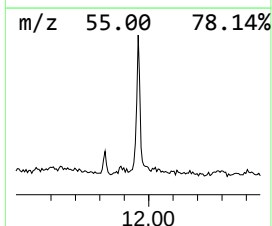
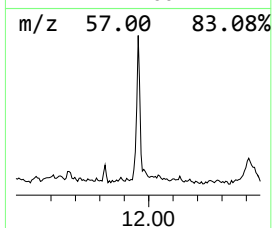
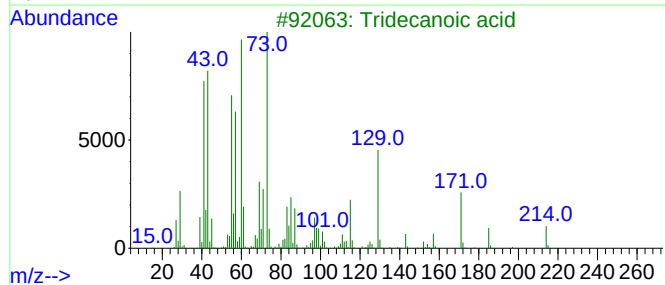
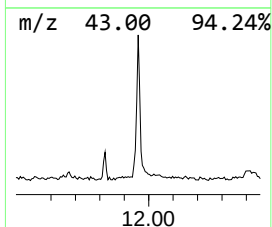
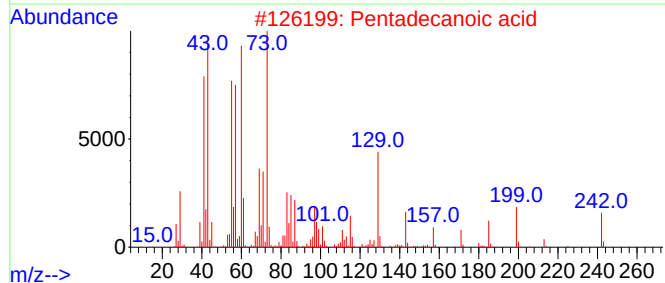
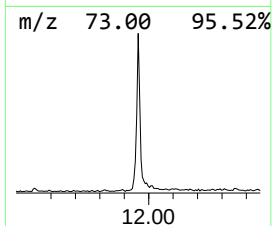
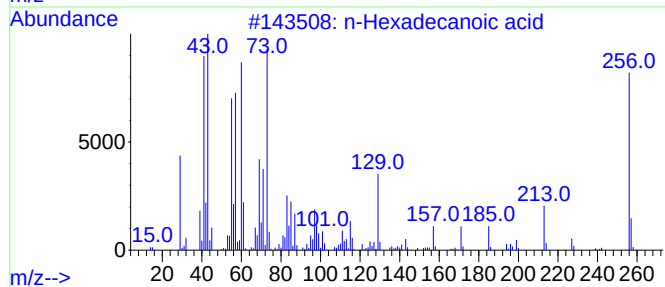
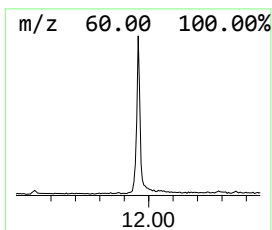
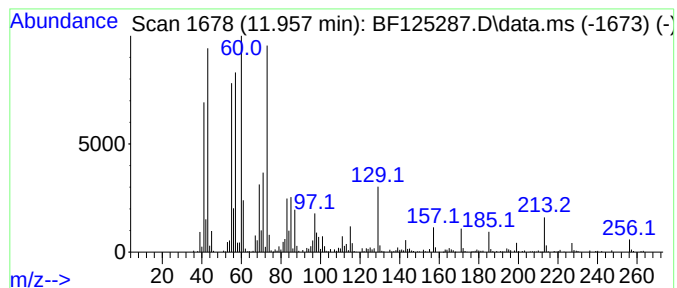
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	9.98 ng	867707	Phenanthrene-d10	11.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	94
3			Tridecanoic acid	214	C13H26O2	000638-53-9	91
4			Dodecanoic acid	200	C12H24O2	000143-07-7	80
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	80



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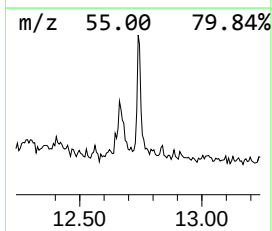
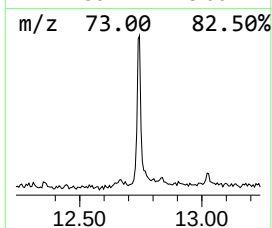
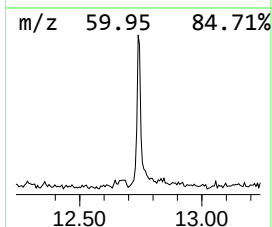
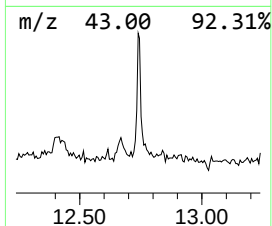
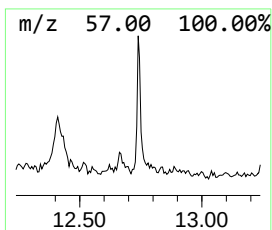
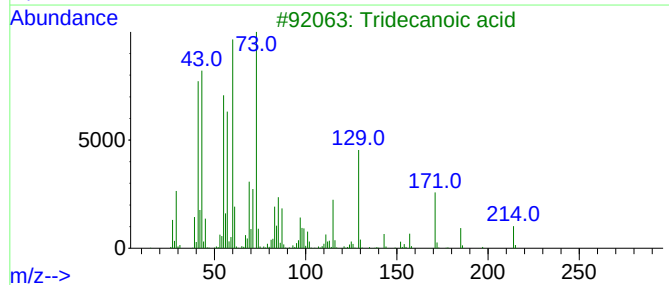
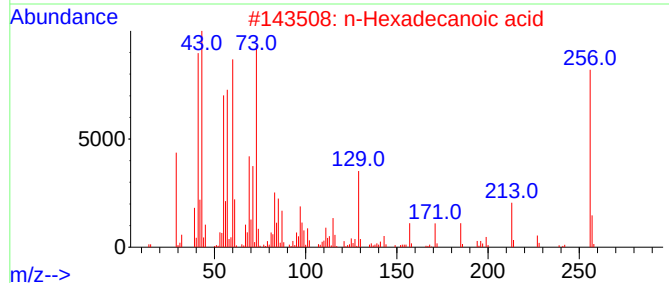
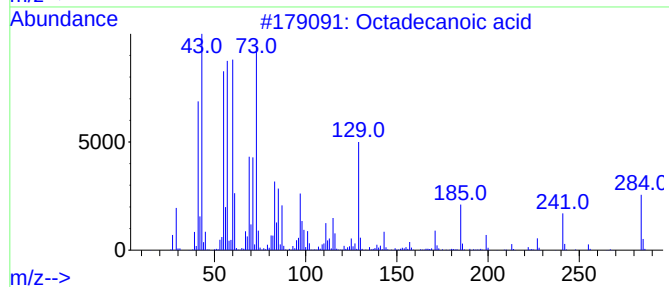
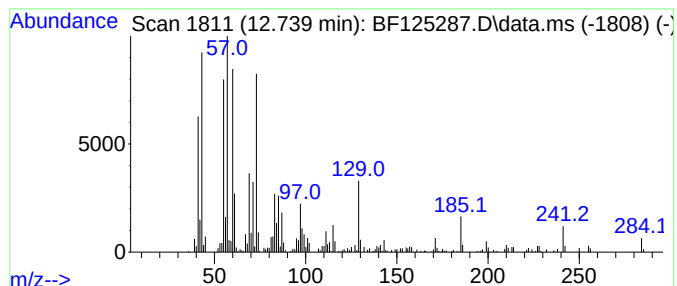
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Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.739	3.70 ng	321520	Phenanthrene-d10	11.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
3			Tridecanoic acid	214	C13H26O2	000638-53-9	76
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72



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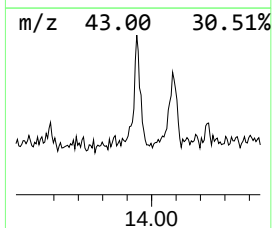
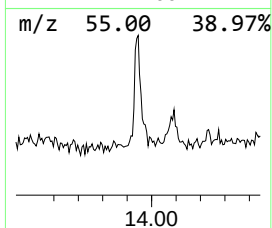
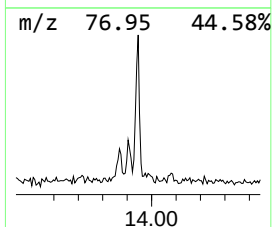
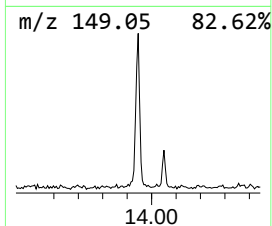
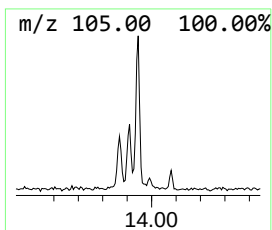
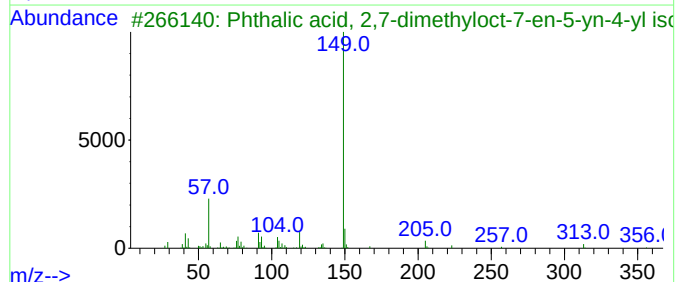
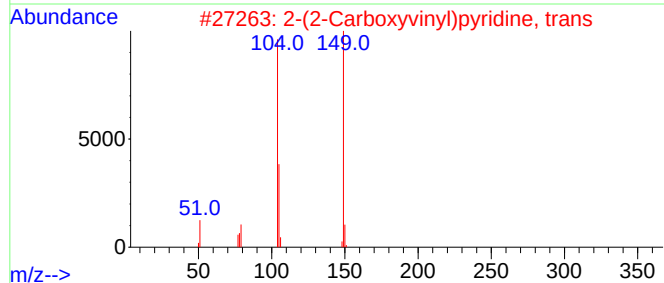
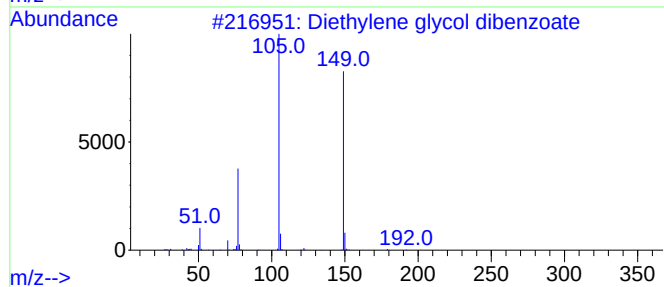
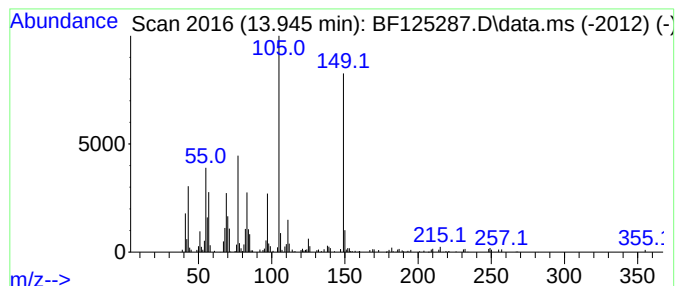
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Diethylene glycol dibenzoate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.945	4.36 ng	344438	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	53
2			2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	38
3			Phthalic acid, 2,7-dimethyloct-7...	356	C22H28O4	1000315-49-7	35
4			Phthalic acid, 5-methoxy-3-methy...	322	C18H26O5	1010314-88-4	35
5			Benzoic acid, 2-ethylhexyl ester	234	C15H22O2	005444-75-7	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083121\
Data File : BF125287.D
Acq On : 31 Aug 2021 14:21
Operator : JU/CG
Sample : M3561-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OUII-E

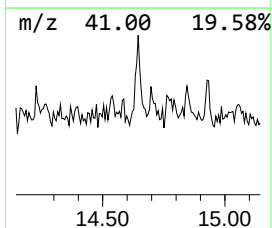
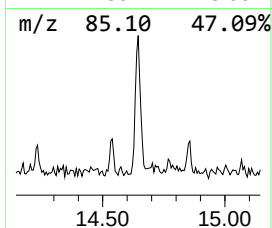
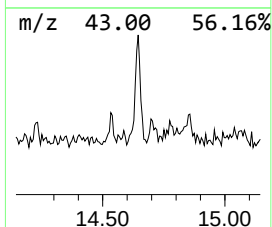
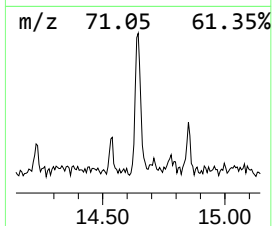
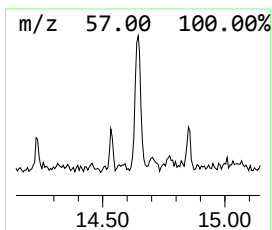
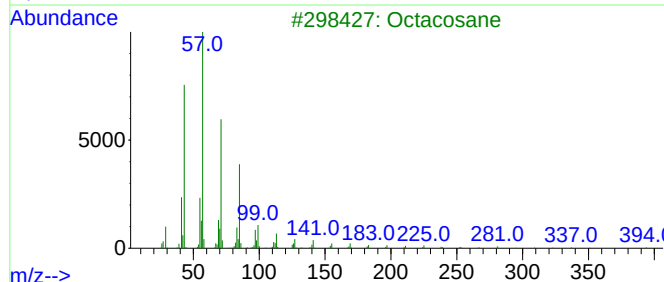
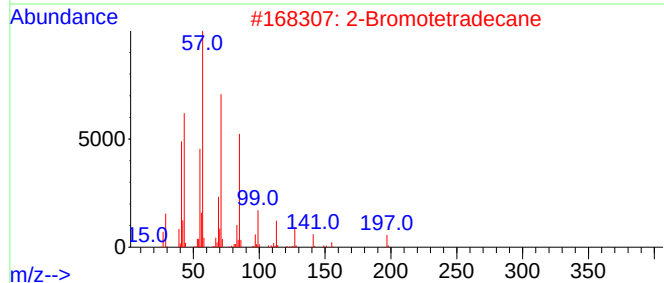
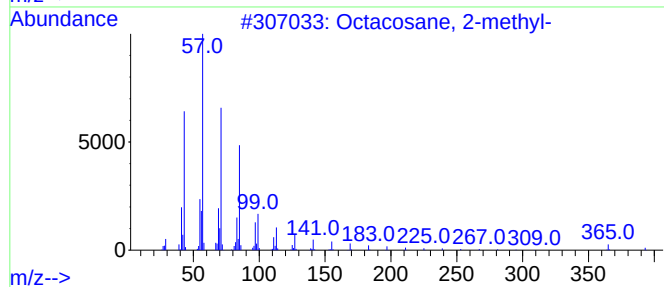
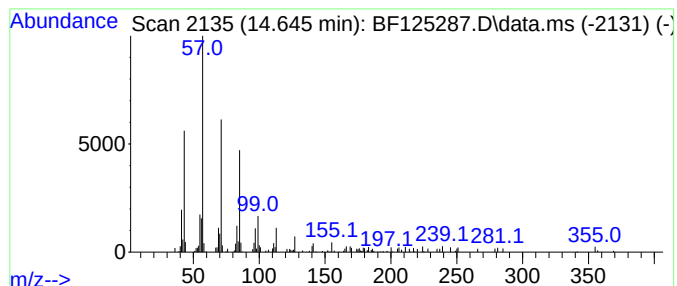
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octacosane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.645	2.18 ng	171851	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
2			2-Bromotetradecane	276	C14H29Br	074036-95-6	86
3			Octacosane	394	C28H58	000630-02-4	86
4			Eicosane, 9-octyl-	394	C28H58	013475-77-9	86
5			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083121\
Data File : BF125287.D
Acq On : 31 Aug 2021 14:21
Operator : JU/CG
Sample : M3561-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OUII-E

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.187	78.3	ng	4128980	1	6.910	1055020	20.0
Ethanol, 2-(2-b...	8.098	12.1	ng	837027	2	8.198	1380030	20.0
unknown9.657	9.657	2.1	ng	177889	3	9.951	1674720	20.0
n-Hexadecanoic ...	11.957	10.0	ng	867707	4	11.439	1739110	20.0
Octadecanoic acid	12.739	3.7	ng	321520	4	11.439	1739110	20.0
Diethylene glyc...	13.945	4.4	ng	344438	5	14.080	1579500	20.0
Octacosane, 2-m...	14.645	2.2	ng	171851	5	14.080	1579500	20.0