

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
 Data File : BF123583.D
 Acq On : 16 Apr 2021 9:42
 Operator : JU/CG
 Sample : PB135740BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB135740BL

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-BF041521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123583.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.204	11	20	26	rVB	253822	344790	3.52%	0.565%
2	5.492	574	579	582	rBV	7910605	8348351	85.20%	13.677%
3	6.498	744	750	753	rBV	7518871	8351324	85.23%	13.681%
4	6.869	809	813	816	rBV	2015728	1587111	16.20%	2.600%
5	7.434	903	909	912	rBV	5520732	5596957	57.12%	9.169%
6	8.151	1026	1031	1035	rBV	2504513	2076060	21.19%	3.401%
7	9.233	1209	1215	1218	rBV	9311306	8804043	89.85%	14.423%
8	9.916	1325	1331	1334	rBV	2388562	2225508	22.71%	3.646%
9	10.704	1459	1465	1468	rBV	6649646	6119986	62.46%	10.026%
10	11.404	1580	1584	1587	rBV	2993538	2348794	23.97%	3.848%
11	12.816	1821	1824	1828	rBV	660854	575083	5.87%	0.942%
12	12.892	1835	1837	1841	rVB	142647	109149	1.11%	0.179%
13	13.004	1850	1856	1859	rBV	9727106	9798989	100.00%	16.053%
14	13.527	1941	1945	1950	rBV	556299	466341	4.76%	0.764%
15	14.051	2030	2034	2047	rVB	2525633	2236134	22.82%	3.663%
16	15.539	2281	2287	2291	rBV	1597186	1938083	19.78%	3.175%
17	15.580	2291	2294	2300	rVB	85365	114635	1.17%	0.188%

Sum of corrected areas: 61041338

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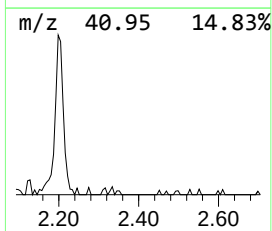
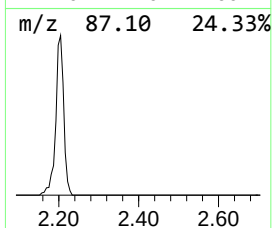
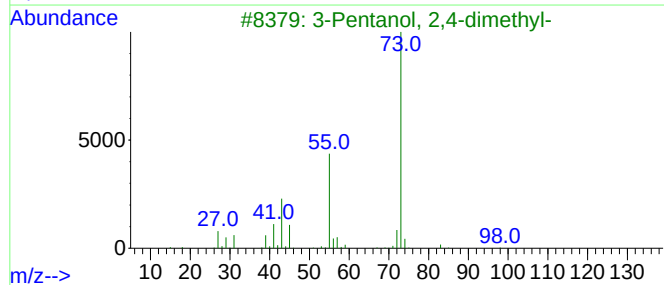
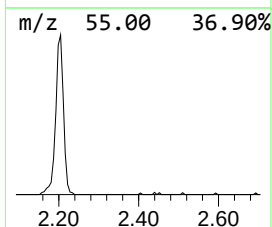
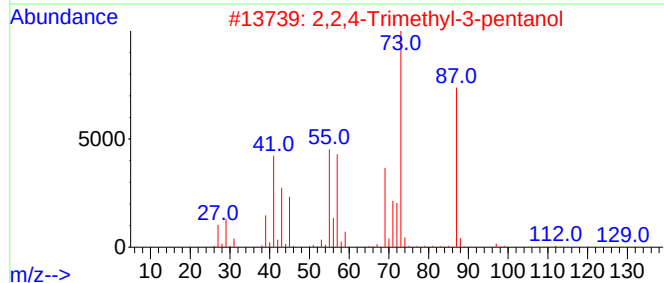
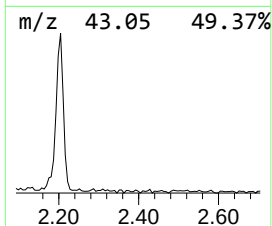
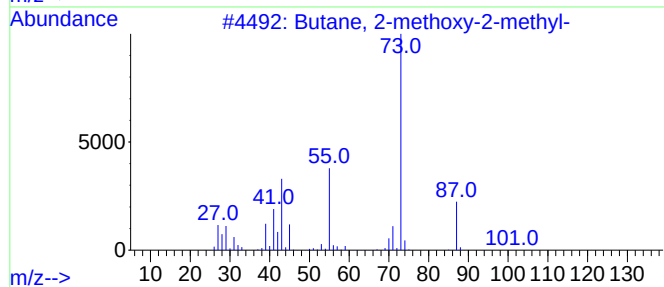
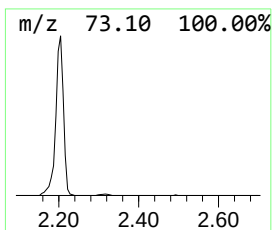
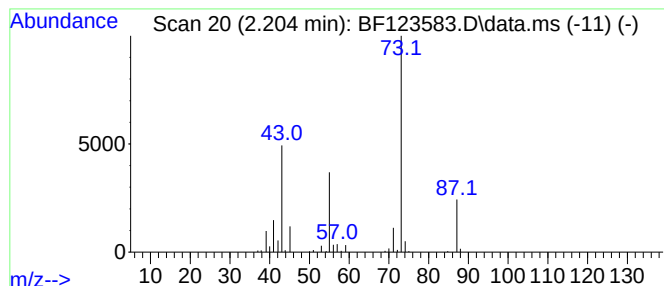
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.204	4.34 ng	344790	1,4-Dichlorobenzene-d4	6.869

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	56
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	17
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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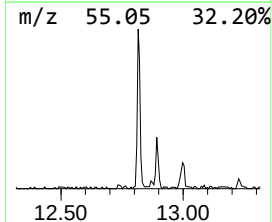
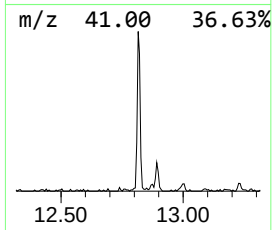
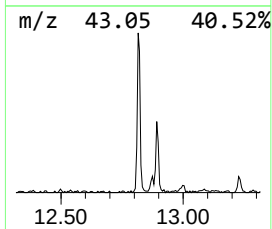
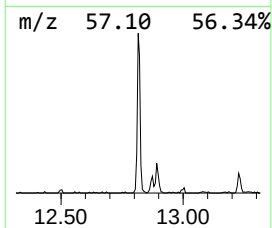
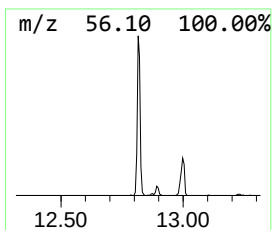
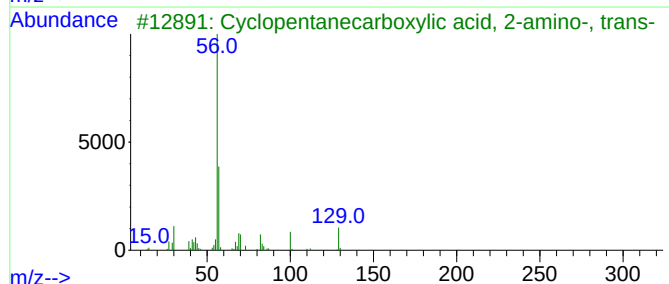
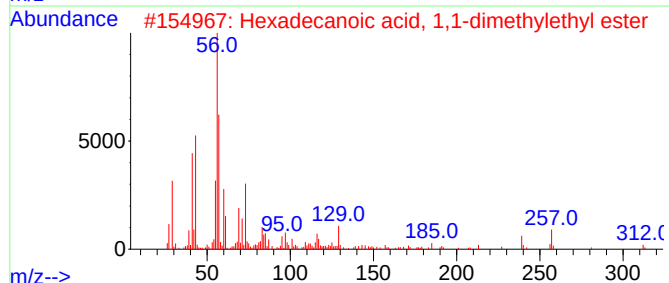
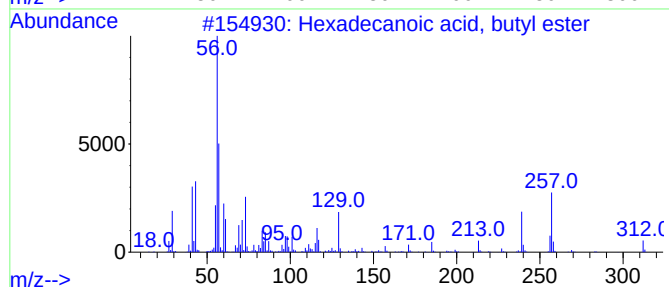
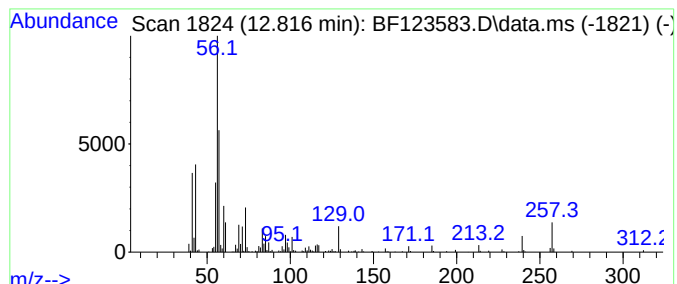
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Peak Number 2 Hexadecanoic acid, butyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.816	5.14 ng	575083	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	83
2			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	83
3			Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	46
4			Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	43
5			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	35



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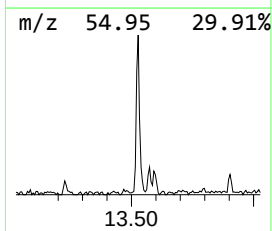
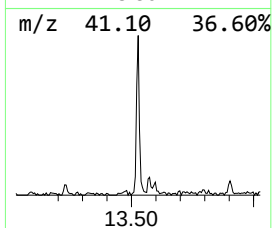
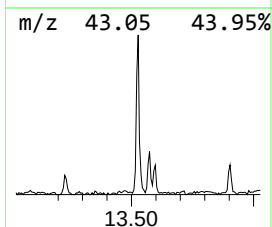
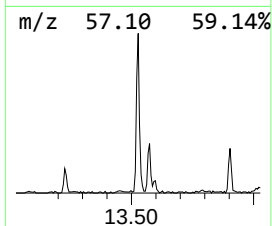
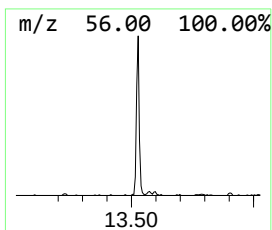
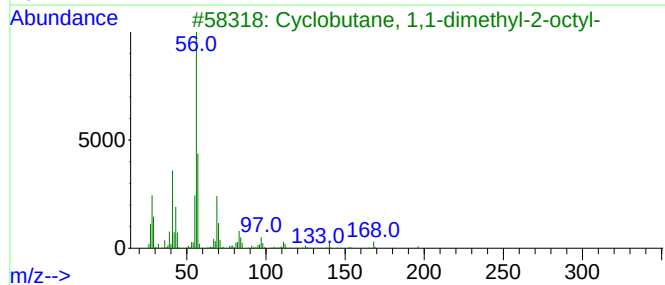
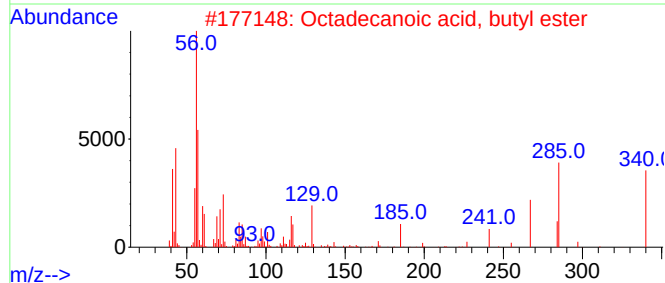
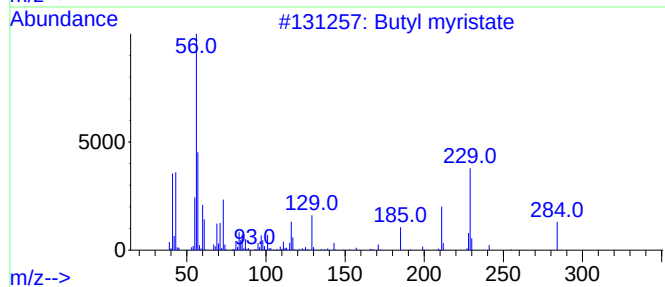
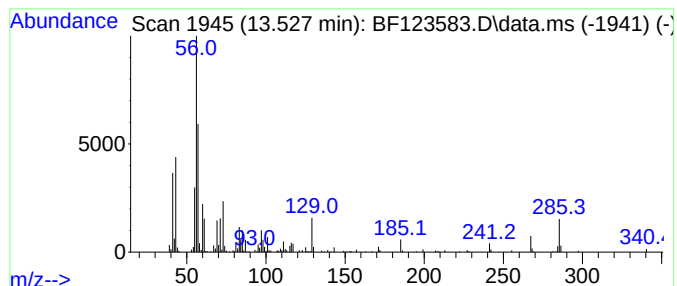
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Butyl myristate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.527	4.17 ng	466341	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butyl myristate	284	C18H36O2	000110-36-1	64
2			Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	49
3			Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38
4			Pentadecane, 8-methylene-	224	C16H32	055668-09-2	37
5			1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	35



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.204	4.3	ng	344790	1	6.869	1587110	20.0
Hexadecanoic ac...	12.816	5.1	ng	575083	5	14.051	2236130	20.0
Butyl myristate	13.527	4.2	ng	466341	5	14.051	2236130	20.0