

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010422\
 Data File : BP008677.D
 Acq On : 04 Jan 2022 23:48
 Operator : CG/JU
 Sample : M5256-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 BU-03-122921

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_P\Methods\8270E-BP122821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008677.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.469	415	422	441	rVB	7378418	11433834	34.65%	5.920%
2	7.063	683	693	709	rBV	7173828	11869276	35.97%	6.145%
3	7.887	826	833	841	rBV	2410019	3856786	11.69%	1.997%
4	9.045	1014	1030	1040	rBV	4727671	8137550	24.66%	4.213%
5	9.957	1177	1185	1197	rBV	230932	586097	1.78%	0.303%
6	10.469	1264	1272	1283	rBV	538438	922774	2.80%	0.478%
7	10.686	1301	1309	1317	rBV	3180267	5735481	17.38%	2.970%
8	12.128	1548	1554	1565	rBV	336750	556752	1.69%	0.288%
9	13.145	1720	1727	1739	rBV	12952200	20785887	62.98%	10.762%
10	13.363	1759	1764	1769	rBV	450734	619417	1.88%	0.321%
11	13.857	1843	1848	1853	rBV	554474	821404	2.49%	0.425%
12	13.945	1858	1863	1867	rBV4	212141	344571	1.04%	0.178%
13	14.369	1930	1935	1940	rVB3	256983	452204	1.37%	0.234%
14	14.433	1940	1946	1950	rBV	603145	869311	2.63%	0.450%
15	14.522	1951	1961	1968	rBV	4629651	8013915	24.28%	4.149%
16	14.780	2001	2005	2012	rVB	295419	468750	1.42%	0.243%
17	14.845	2012	2016	2023	rBV	187099	454613	1.38%	0.235%
18	15.051	2047	2051	2058	rBV2	238457	382672	1.16%	0.198%
19	15.380	2103	2107	2111	rBV	547029	701721	2.13%	0.363%
20	16.010	2208	2214	2222	rBV	9675575	14228650	43.11%	7.367%
21	16.245	2250	2254	2257	rBV	693736	925208	2.80%	0.479%
22	17.045	2386	2390	2394	rBV	343105	474950	1.44%	0.246%
23	17.098	2396	2399	2408	rVB3	373170	627953	1.90%	0.325%
24	17.269	2423	2428	2432	rBV	5239610	7549915	22.88%	3.909%
25	17.310	2432	2435	2443	rVB	1780821	2524365	7.65%	1.307%
26	17.780	2512	2515	2519	rBV	344602	382520	1.16%	0.198%
27	18.163	2577	2580	2588	rVB2	1274343	2037051	6.17%	1.055%
28	19.274	2765	2769	2776	rVB	3370973	4450099	13.48%	2.304%
29	19.392	2786	2789	2796	rVB2	520819	696456	2.11%	0.361%
30	19.627	2825	2829	2837	rVB	2319336	3423055	10.37%	1.772%
31	19.827	2858	2863	2873	rVB	17257947	22238958	67.39%	11.514%
32	20.904	3043	3046	3050	rBV	2072788	2310510	7.00%	1.196%
33	21.062	3070	3073	3079	rVB3	1566363	1982548	6.01%	1.026%
34	21.351	3116	3122	3126	rBV2	5066084	7851709	23.79%	4.065%
35	21.474	3137	3143	3156	rBV	20455447	33001638	100.00%	17.087%
36	21.992	3228	3231	3236	rVB2	1468961	1867307	5.66%	0.967%

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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_P\Methods\8270E-BP122821.M
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37	23.045	3406	3410	3415	rBV2	1536636	2448775	7.42%	1.268%
38	23.774	3529	3534	3544	rVB2	3352404	7106091	21.53%	3.679%

Sum of corrected areas: 193140773

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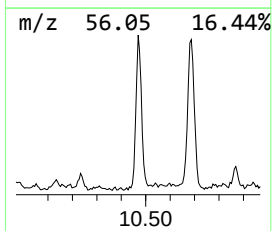
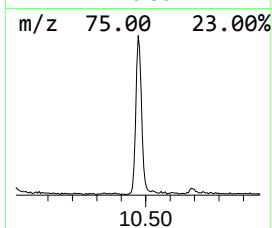
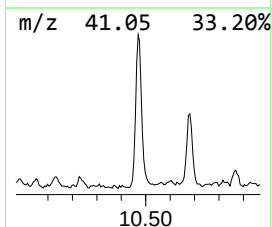
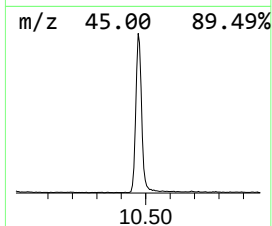
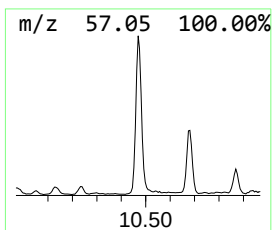
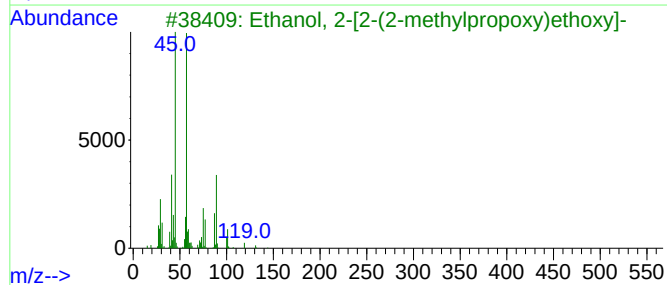
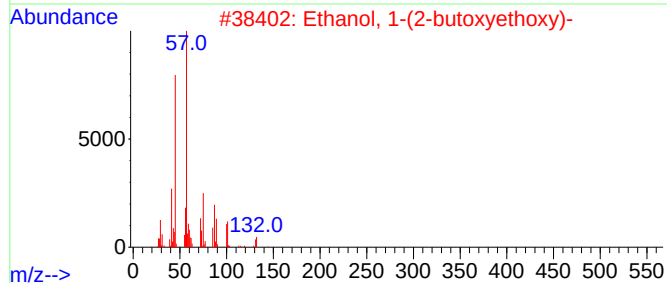
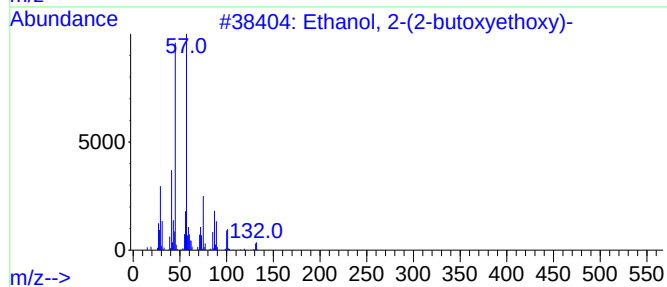
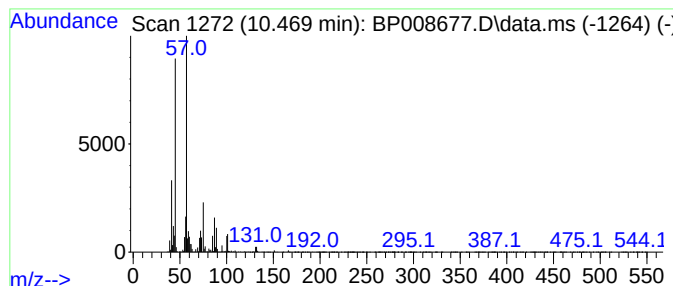
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP122821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.469	3.22 ng	922774	Naphthalene-d8	10.692

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	91
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
4			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50
5			Hexaethylene glycol	282	C12H26O7	002615-15-8	47



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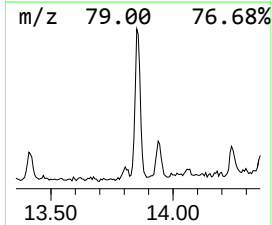
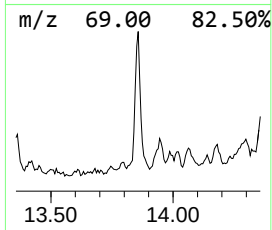
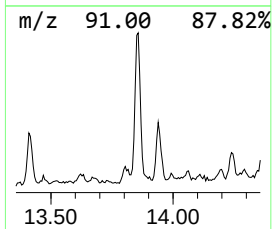
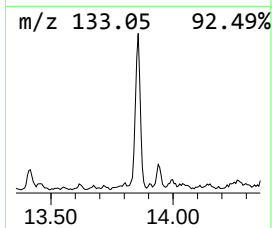
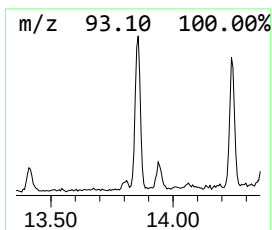
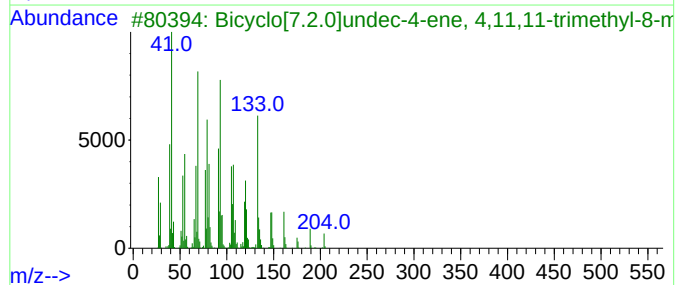
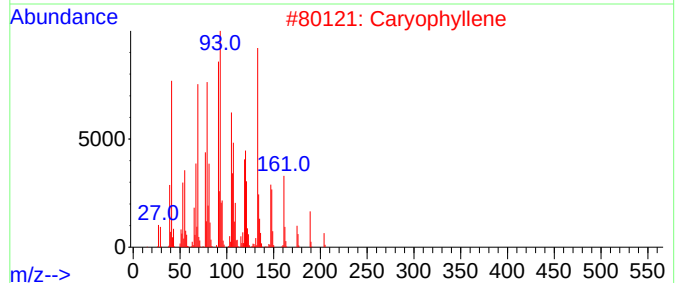
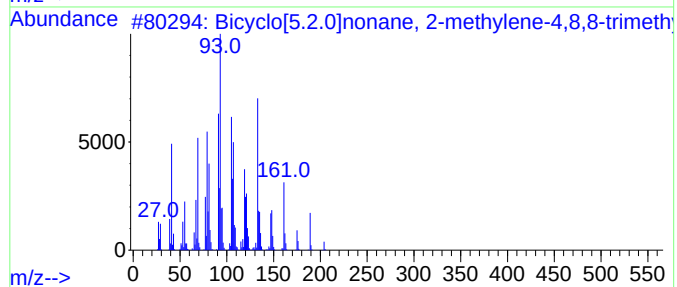
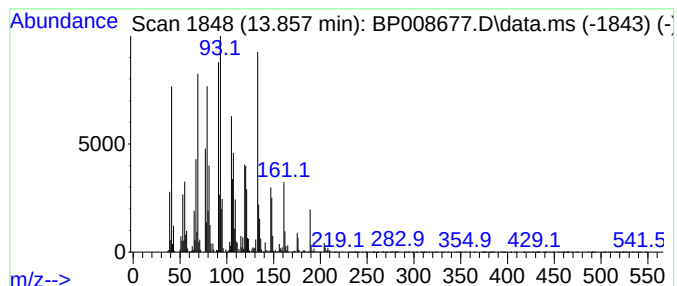
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Bicyclo[5.2.0]nonane, 2-met... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	2.05 ng	821404	Acenaphthene-d10	14.522

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[5.2.0]nonane, 2-methylen...	204	C15H24	242794-76-9	96
2			Caryophyllene	204	C15H24	000087-44-5	94
3			Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	000118-65-0	87
4			Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	013877-93-5	70
5			Cyclohexane, 1,5-diethenyl-3-met...	162	C12H18	074742-35-1	55



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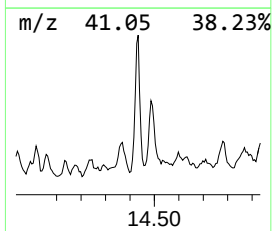
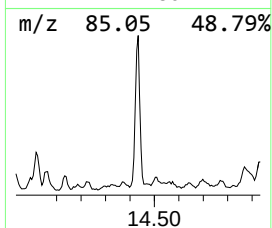
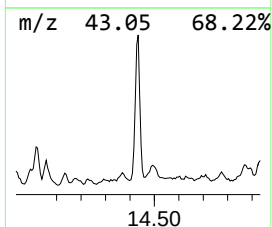
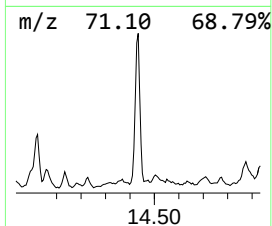
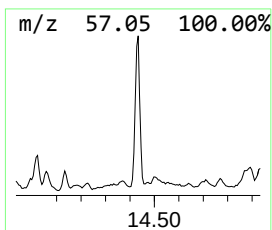
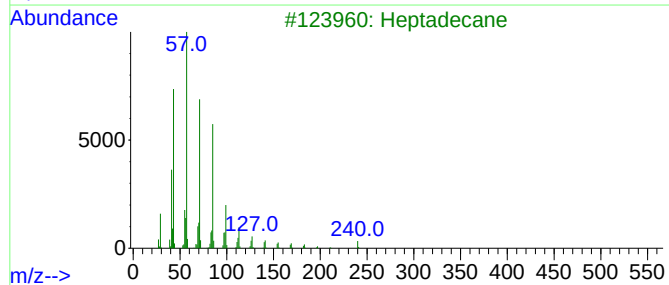
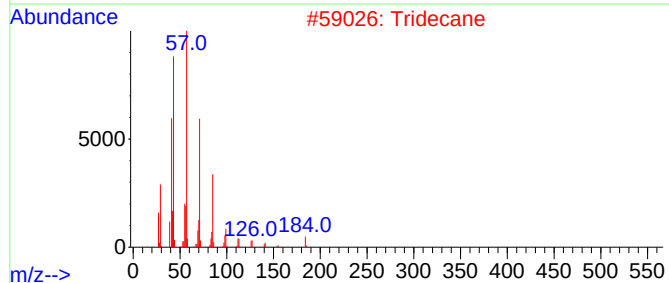
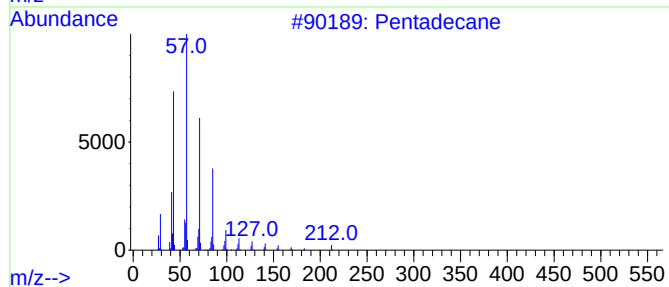
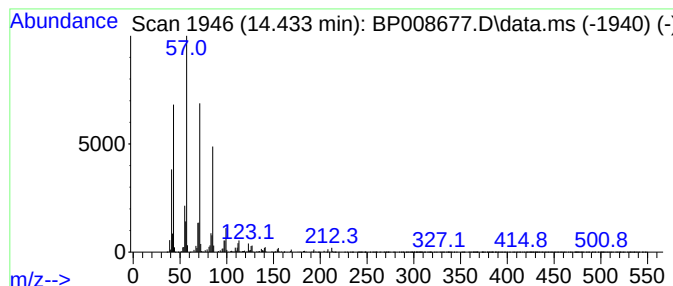
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Pentadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.433	2.17 ng	869311	Acenaphthene-d10	14.522

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecane	212	C15H32	000629-62-9	95
2			Tridecane	184	C13H28	000629-50-5	89
3			Heptadecane	240	C17H36	000629-78-7	87
4			Tetradecane	198	C14H30	000629-59-4	87
5			Nonadecane	268	C19H40	000629-92-5	87



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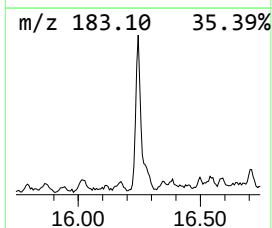
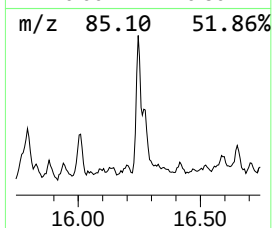
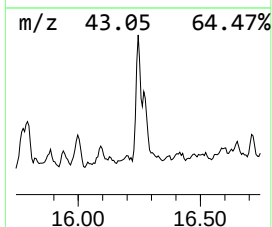
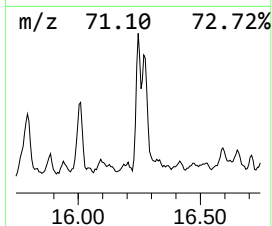
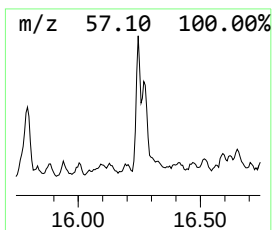
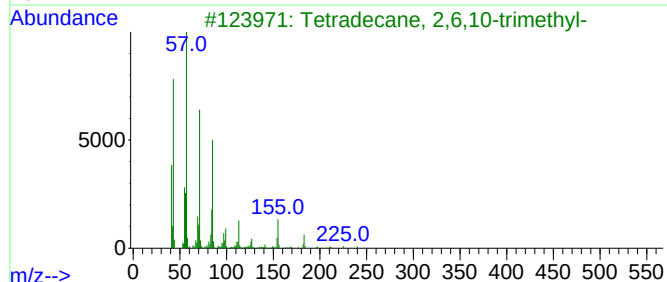
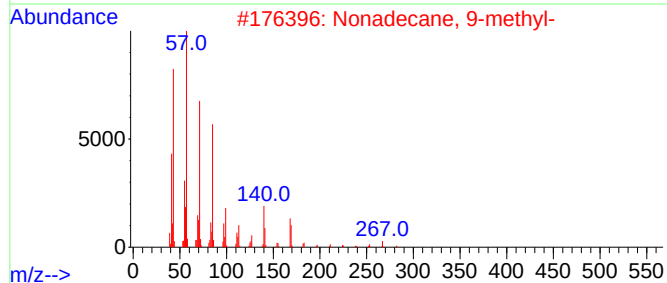
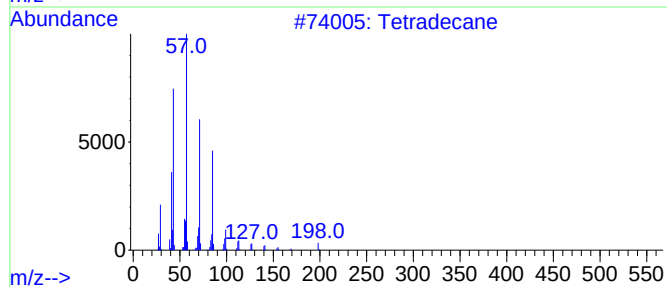
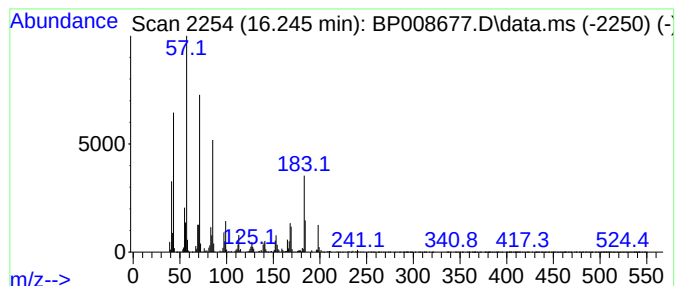
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Tetradecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.245	2.45 ng	925208	Phenanthrene-d10	17.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	83
2			Nonadecane, 9-methyl-	282	C20H42	013287-24-6	76
3			Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	70
4			Nonadecane	268	C19H40	000629-92-5	64
5			Hexacosane	366	C26H54	000630-01-3	64



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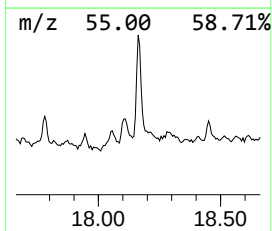
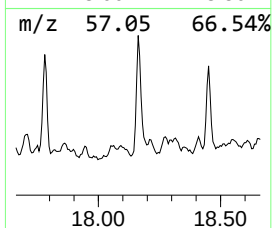
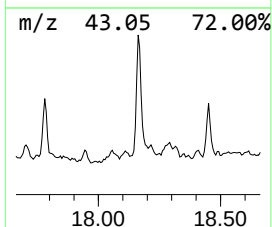
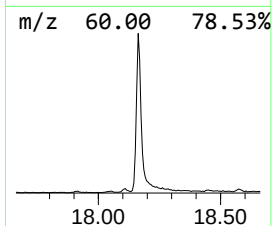
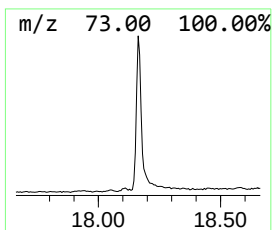
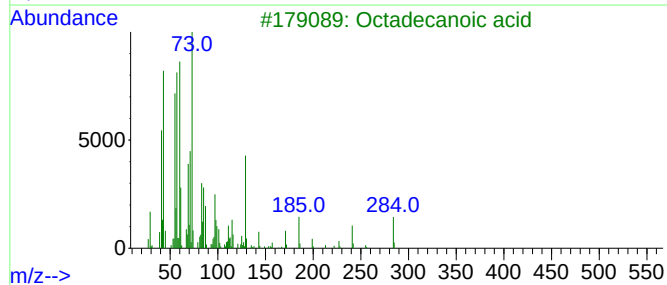
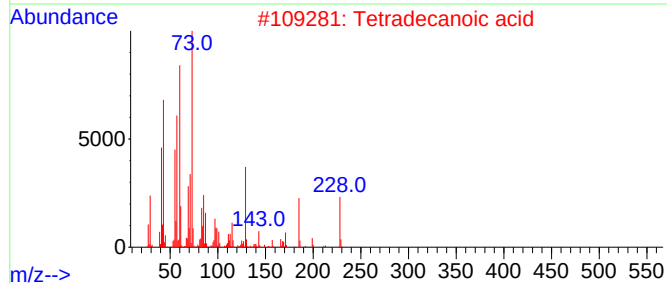
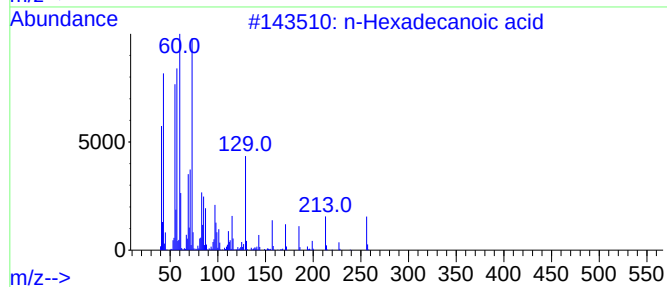
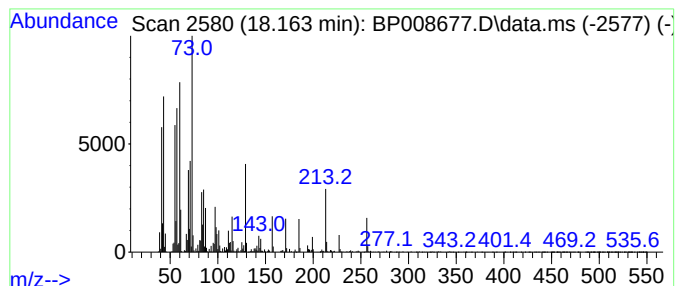
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP122821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.163	5.40 ng	2037050	Phenanthrene-d10	17.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3			Octadecanoic acid	284	C18H36O2	000057-11-4	87
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			Tridecanoic acid	214	C13H26O2	000638-53-9	86



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BU-03-122921

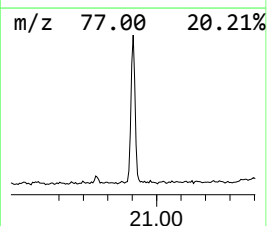
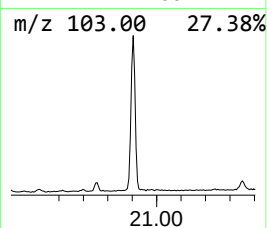
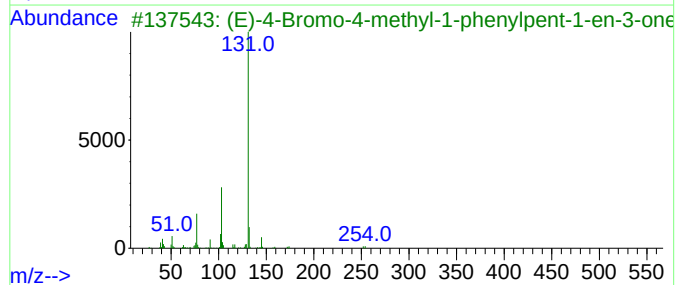
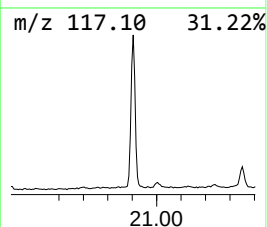
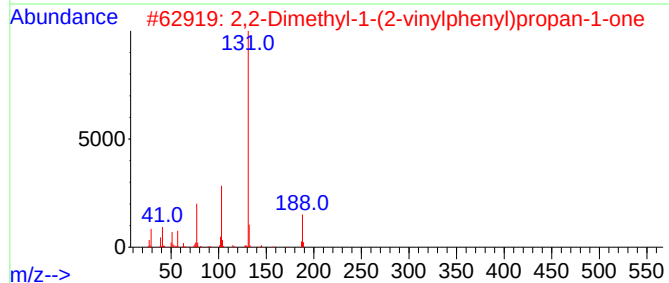
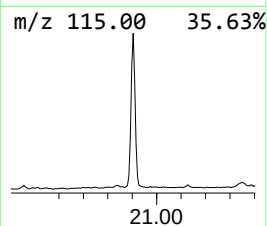
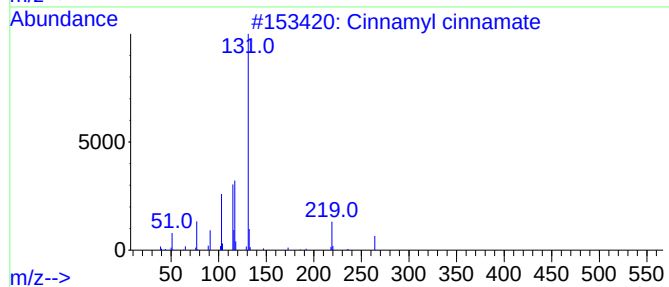
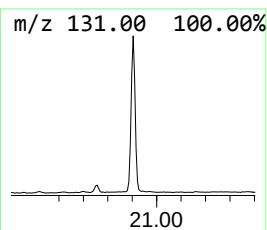
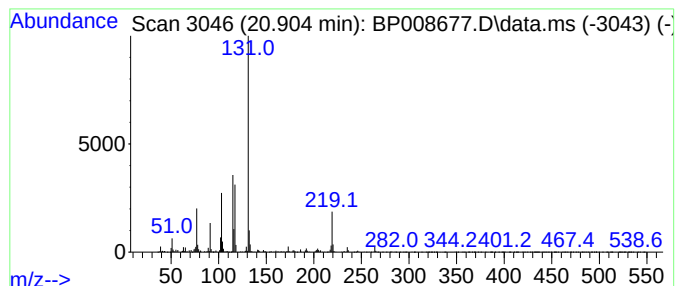
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cinnamyl cinnamate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.904	5.89 ng	2310510	Chrysene-d12	21.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cinnamyl cinnamate	264	C18H16O2	000122-69-0	86
2			2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	52
3			(E)-4-Bromo-4-methyl-1-phenylpen...	252	C12H13BrO	1000443-02-8	50
4			N-(p-Vinylbenzoyl)-1-alanine	219	C12H13NO3	139184-60-4	50
5			N-(4-Fluorophenyl)-3-phenyl-2-pr...	337	C17H11F4NO2	1000492-37-5	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010422\
Data File : BP008677.D
Acq On : 04 Jan 2022 23:48
Operator : CG/JU
Sample : M5256-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BU-03-122921

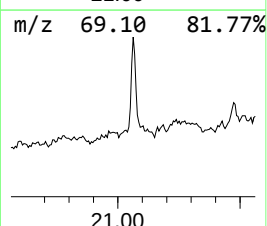
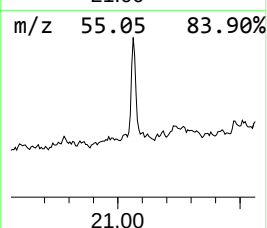
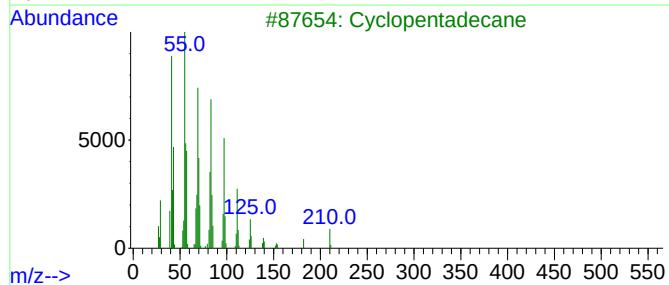
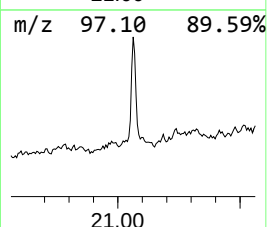
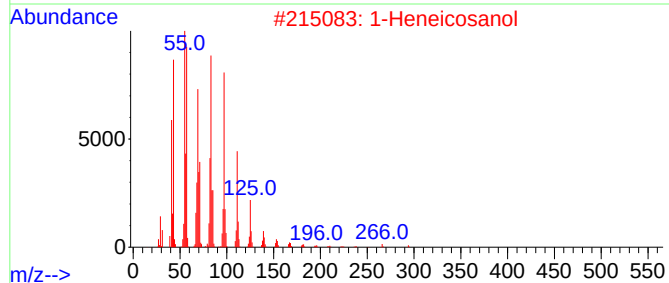
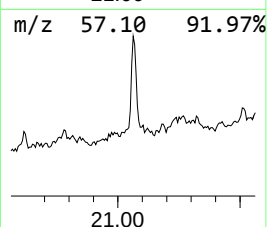
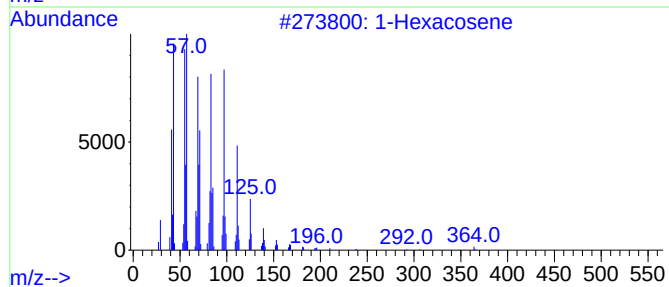
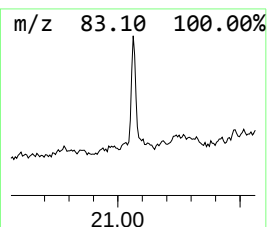
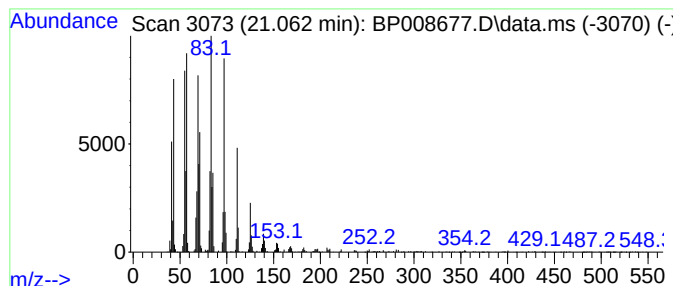
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Hexacosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.062	5.05 ng	1982550	Chrysene-d12	21.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexacosene	364	C26H52	018835-33-1	95
2			1-Heneicosanol	312	C21H44O	015594-90-8	95
3			Cyclopentadecane	210	C15H30	000295-48-7	94
4			2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
5			Behenic alcohol	326	C22H46O	000661-19-8	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010422\
Data File : BP008677.D
Acq On : 04 Jan 2022 23:48
Operator : CG/JU
Sample : M5256-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BU-03-122921

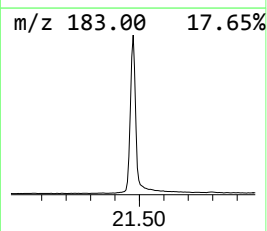
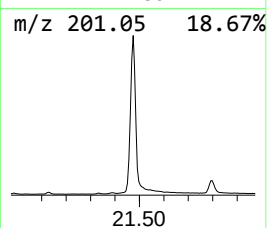
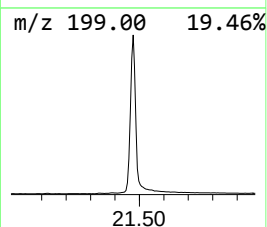
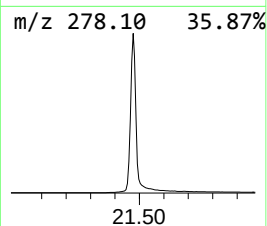
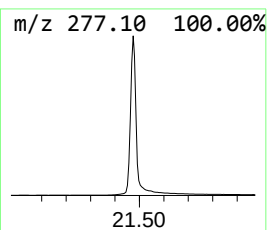
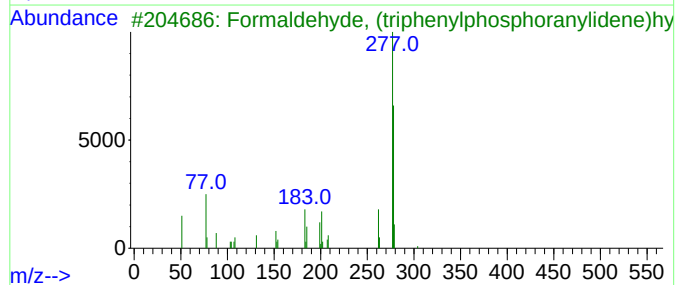
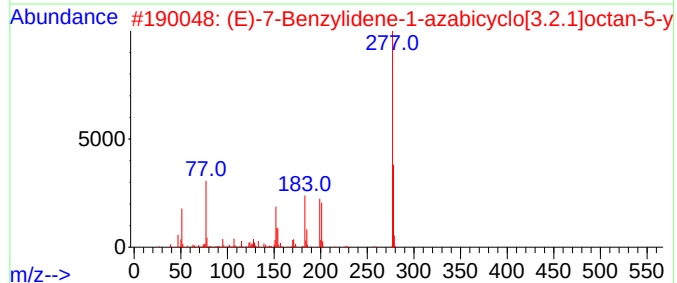
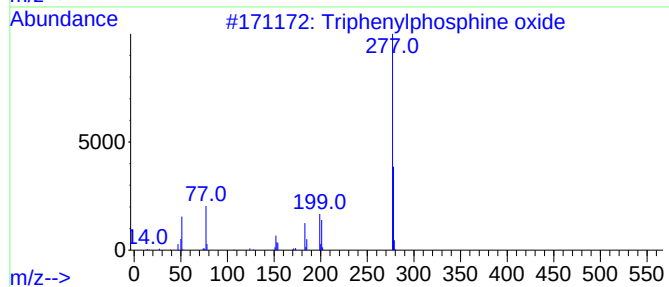
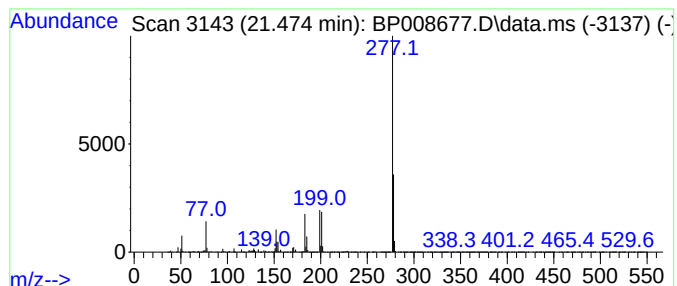
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.474	84.06 ng	33001600	Chrysene-d12	21.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	96
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	91
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	47
4			5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	28
5			Thiophene-3-carbonitrile, 4-(4-m...	277	C13H11NO2S2	1000268-75-0	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010422\
Data File : BP008677.D
Acq On : 04 Jan 2022 23:48
Operator : CG/JU
Sample : M5256-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BU-03-122921

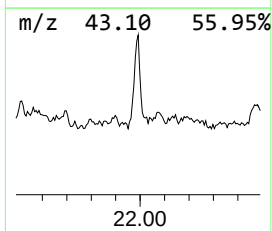
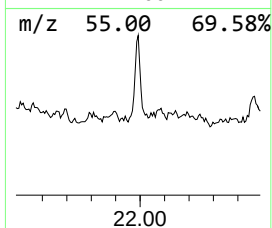
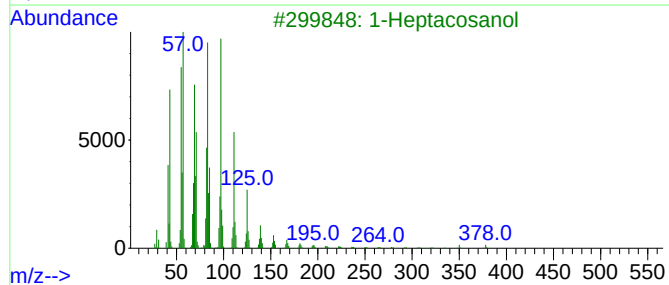
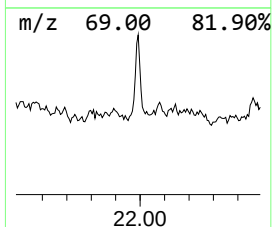
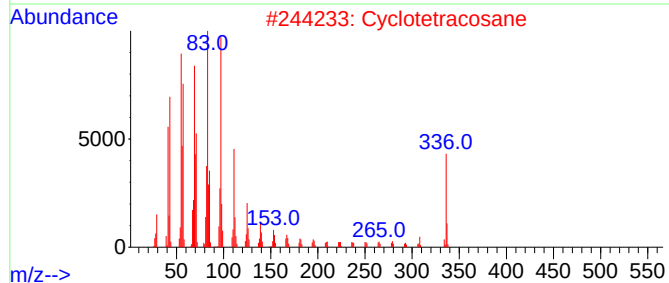
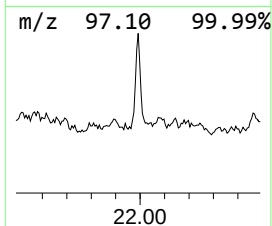
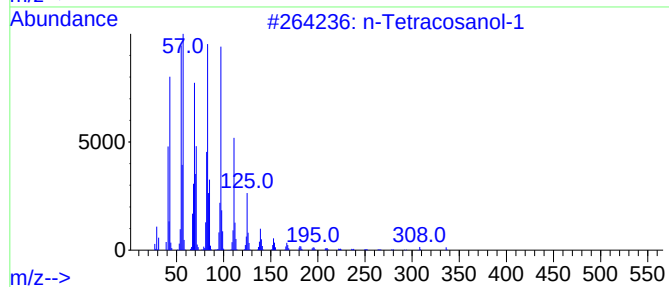
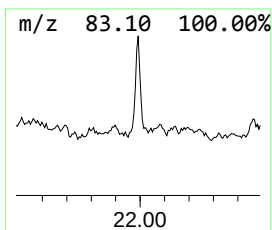
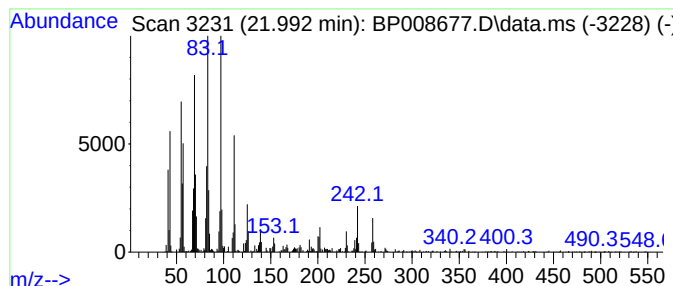
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 n-Tetracosanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.992	4.76 ng	1867310	Chrysene-d12	21.351

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Tetracosanol-1	354	C24H50O	000506-51-4	93
2		Cyclotetracosane	336	C24H48	000297-03-0	93
3		1-Heptacosanol	396	C27H56O	002004-39-9	93
4		n-Nonadecanol-1	284	C19H40O	001454-84-8	87
5		1-Heneicosanol	312	C21H44O	015594-90-8	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010422\
Data File : BP008677.D
Acq On : 04 Jan 2022 23:48
Operator : CG/JU
Sample : M5256-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BU-03-122921

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP122821.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
Ethanol, 2-(2-b...	10.469	3.2	ng	922774	2	10.692	5735480	20.0
Bicyclo[5.2.0]n...	13.857	2.0	ng	821404	3	14.522	8013920	20.0
Pentadecane	14.433	2.2	ng	869311	3	14.522	8013920	20.0
Tetradecane	16.245	2.5	ng	925208	4	17.269	7549920	20.0
n-Hexadecanoic ...	18.163	5.4	ng	2037050	4	17.269	7549920	20.0
Cinnamyl cinnamate	20.904	5.9	ng	2310510	5	21.351	7851710	20.0
1-Hexacosene	21.062	5.0	ng	1982550	5	21.351	7851710	20.0
Triphenylphosph...	21.474	84.1	ng	33001600	5	21.351	7851710	20.0
n-Tetracosanol-1	21.992	4.8	ng	1867310	5	21.351	7851710	20.0