

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011022\
 Data File : BP008758.D
 Acq On : 10 Jan 2022 19:47
 Operator : CG/JU
 Sample : N1054-15
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 20220023-CAPE-5-MODIFIED-ELUTRIATE

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-BP010622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008758.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.076	10	15	20	rBV	3125296	3697462	22.26%	5.053%
2	4.987	334	340	352	rVB	166786	252876	1.52%	0.346%
3	5.452	412	419	437	rBV	2922442	4398940	26.49%	6.012%
4	7.040	681	689	706	rBV	2313927	3856922	23.22%	5.271%
5	7.869	823	830	838	rBV	832634	1343883	8.09%	1.837%
6	9.028	1013	1027	1048	rBV	2674058	4662103	28.07%	6.372%
7	10.452	1261	1269	1287	rBV	233264	511181	3.08%	0.699%
8	10.669	1298	1306	1316	rBV	998117	1729020	10.41%	2.363%
9	13.128	1717	1724	1746	rBV	7520541	12118046	72.96%	16.562%
10	14.504	1951	1958	1979	rBV	1292113	2193872	13.21%	2.998%
11	15.993	2205	2211	2231	rBV	5829714	9760279	58.77%	13.339%
12	17.257	2419	2426	2438	rBV	1691786	2581105	15.54%	3.528%
13	18.151	2573	2578	2586	rBV	343329	513665	3.09%	0.702%
14	19.386	2783	2788	2799	rBV	297065	511362	3.08%	0.699%
15	19.816	2855	2861	2875	rBV	13062654	16608237	100.00%	22.698%
16	20.610	2993	2996	2999	rVB	192835	199066	1.20%	0.272%
17	21.063	3068	3073	3079	rBV2	589297	866785	5.22%	1.185%
18	21.345	3116	3121	3133	rBV	2226207	3052685	18.38%	4.172%
19	21.504	3145	3148	3152	rVB	266758	282744	1.70%	0.386%
20	21.969	3224	3227	3233	rVB	255846	317081	1.91%	0.433%
21	22.469	3309	3312	3319	rVB3	331046	525962	3.17%	0.719%
22	23.769	3526	3533	3544	rVB2	1414808	3185766	19.18%	4.354%

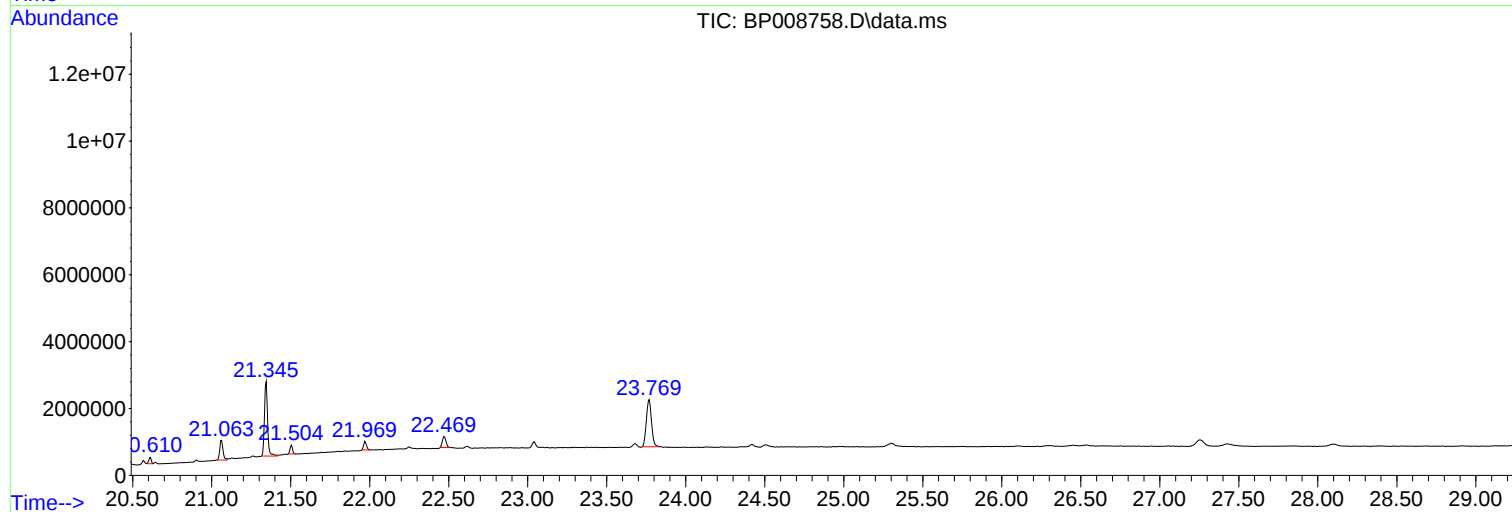
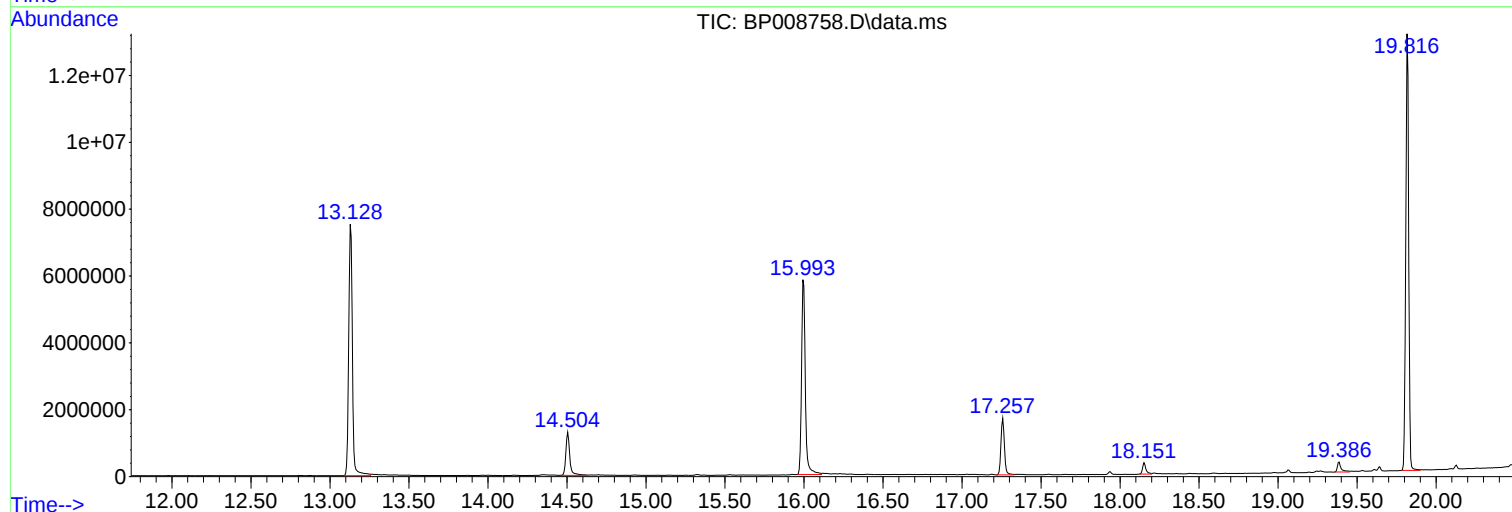
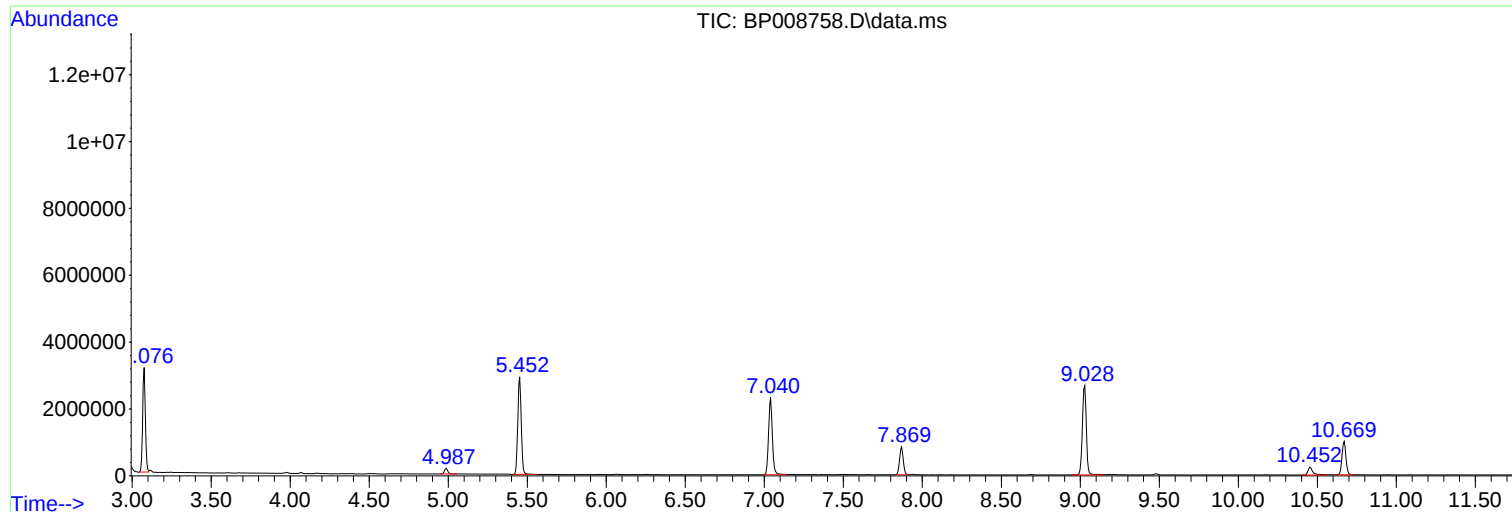
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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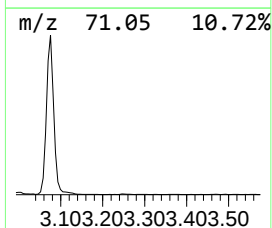
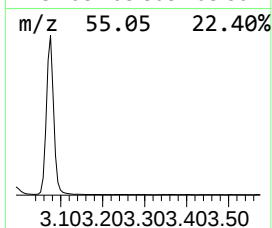
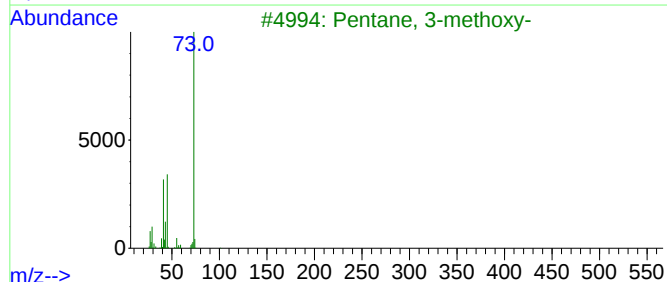
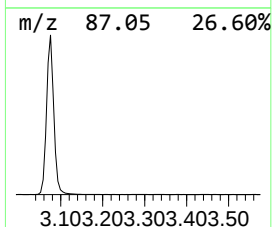
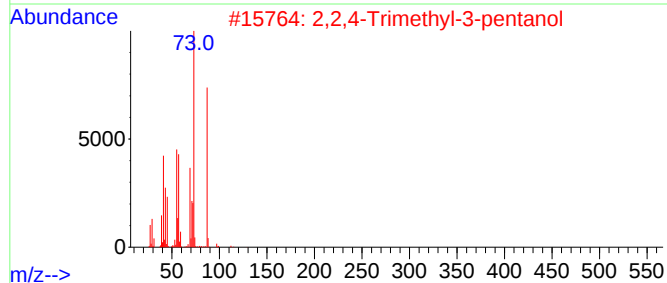
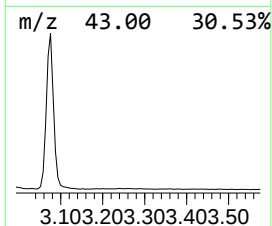
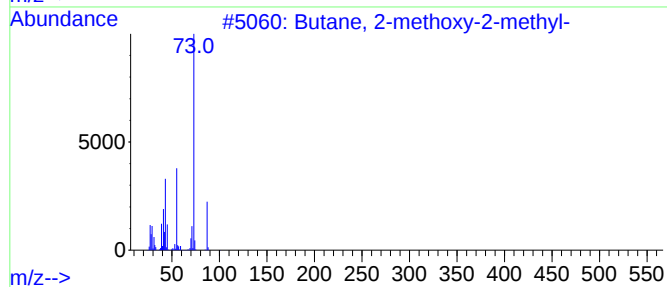
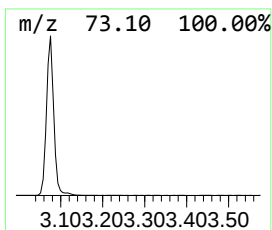
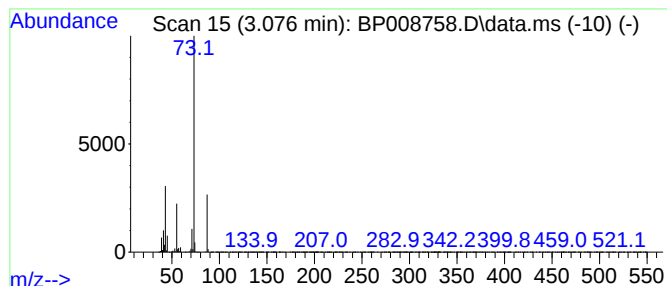
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
3.076	55.03 ng	3697460	1,4-Dichlorobenzene-d4	7.869

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	39
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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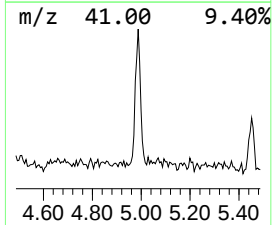
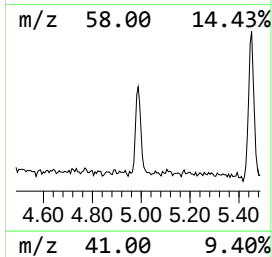
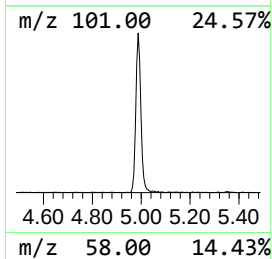
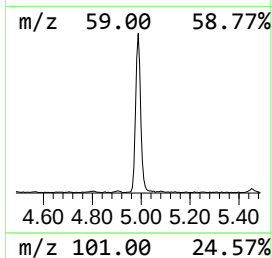
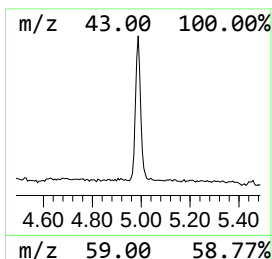
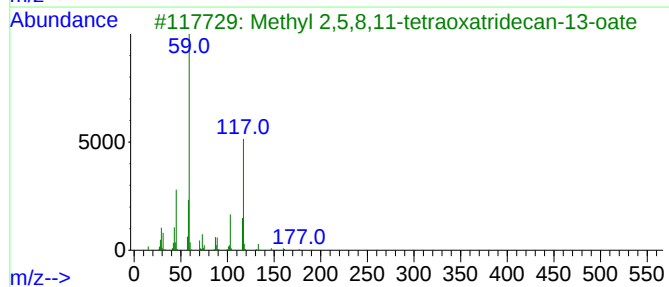
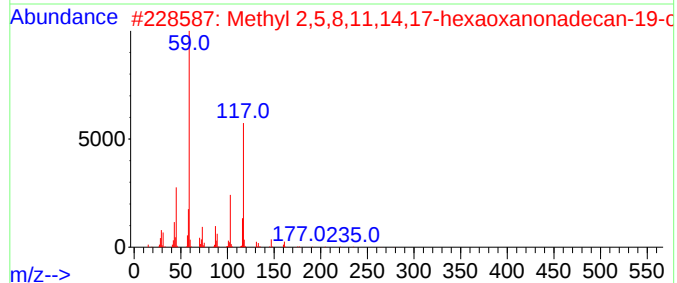
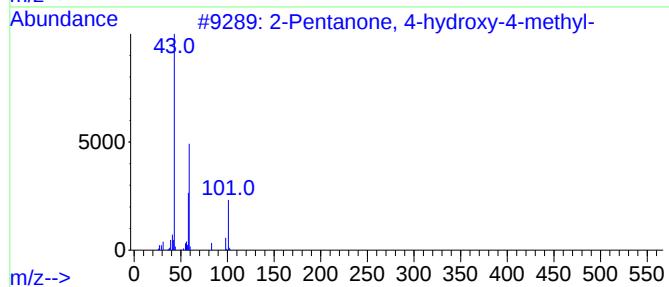
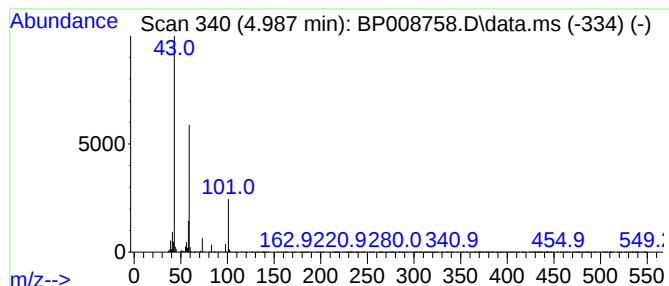
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.987	3.76 ng	252876	1,4-Dichlorobenzene-d4	7.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Methyl 2,5,8,11,14,17-hexaoxonon...	324	C14H28O8	1000366-81-4	37
3			Methyl 2,5,8,11-tetraoxatridecan...	236	C10H20O6	1000366-78-2	32
4			Dimethadione	129	C5H7NO3	000695-53-4	28
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25



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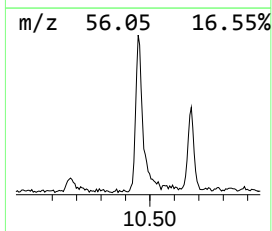
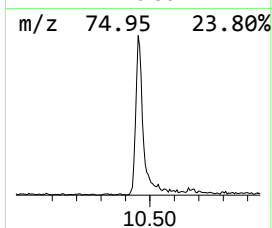
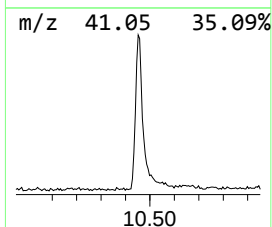
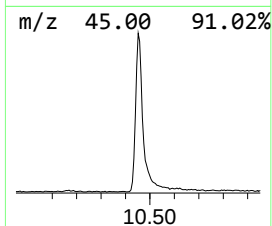
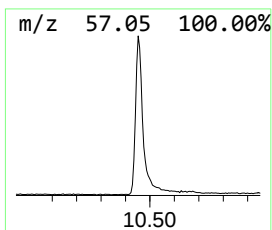
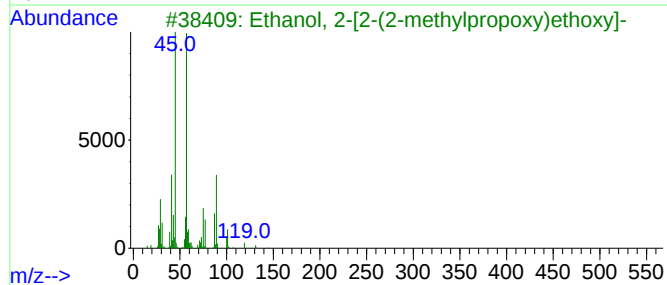
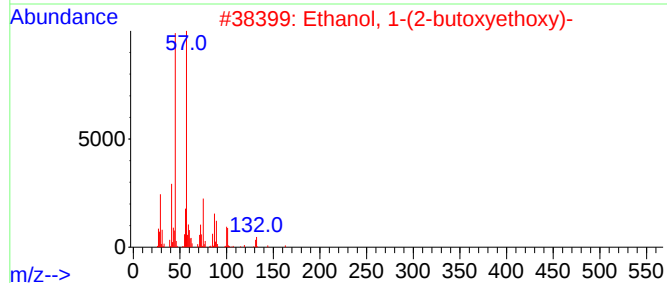
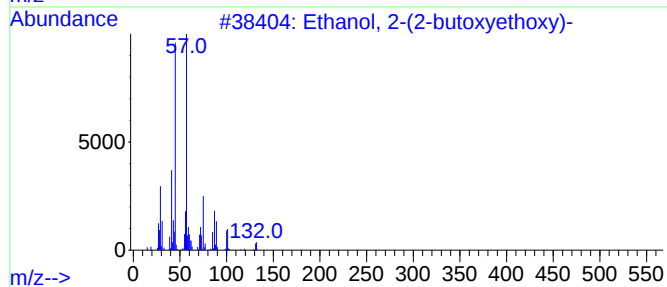
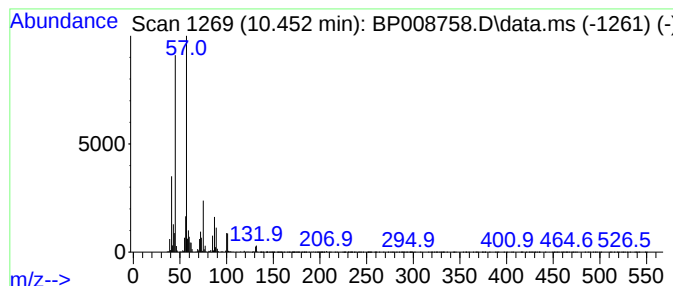
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.452	5.91 ng	511181	Naphthalene-d8	10.669

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	72
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
5			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50



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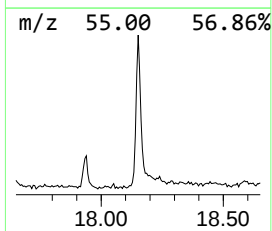
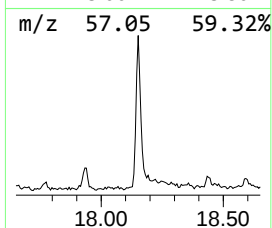
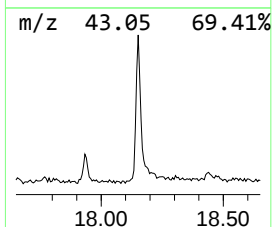
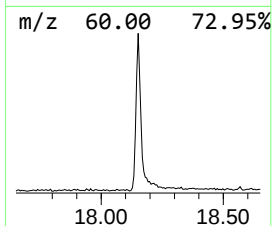
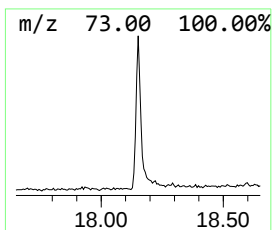
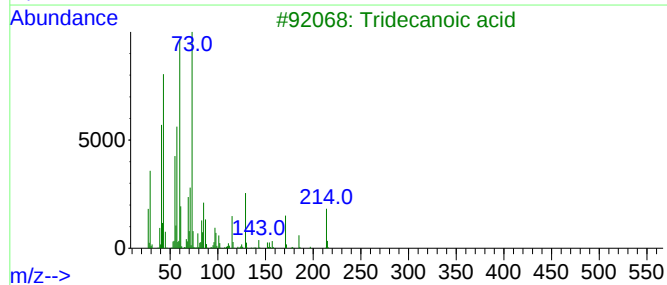
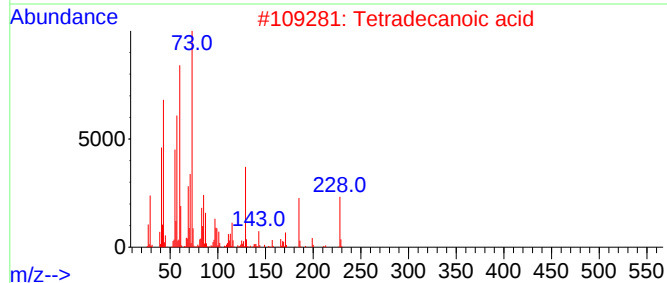
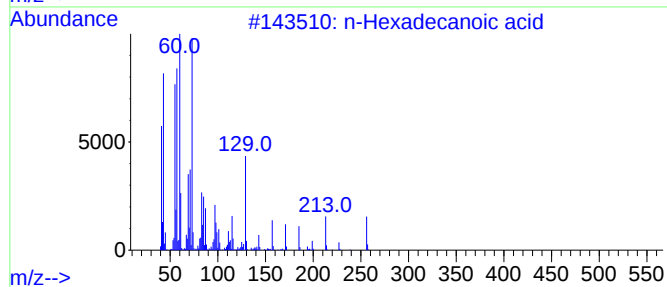
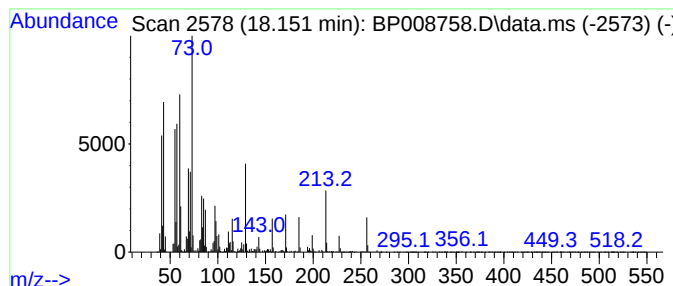
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.151	3.98 ng	513665	Phenanthrene-d10	17.257

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	90
3			Tridecanoic acid	214	C13H26O2	000638-53-9	90
4			Octadecanoic acid	284	C18H36O2	000057-11-4	81
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	74



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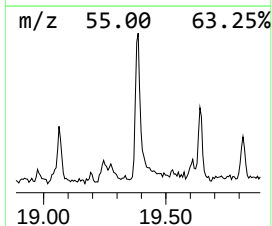
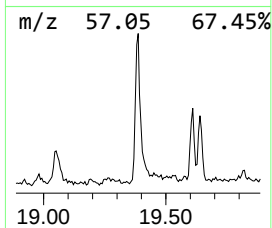
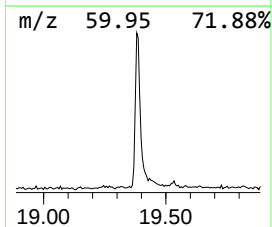
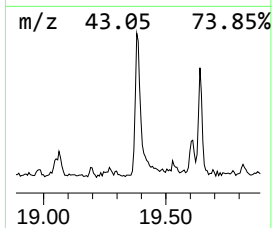
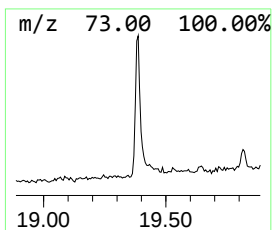
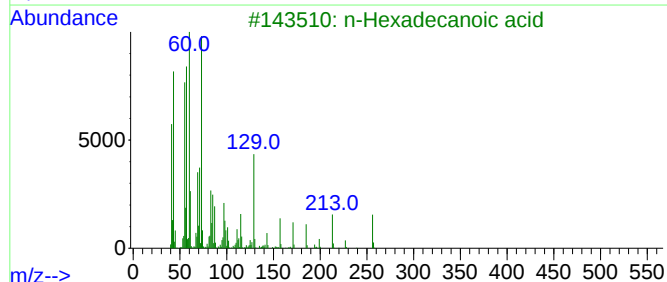
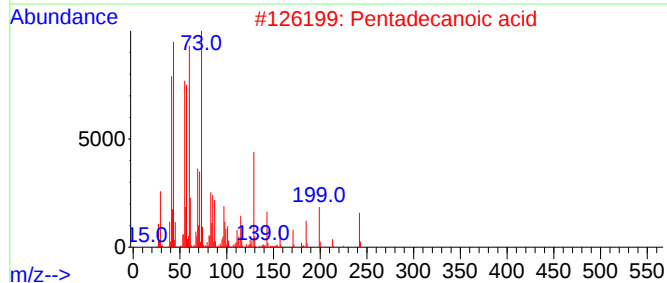
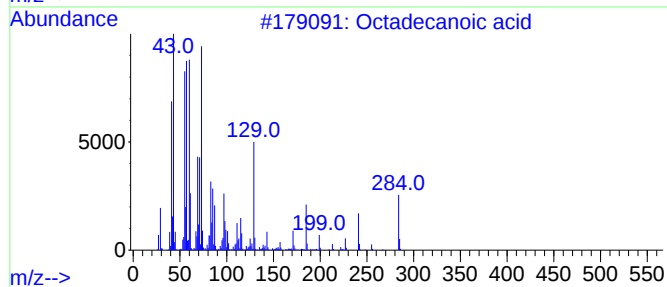
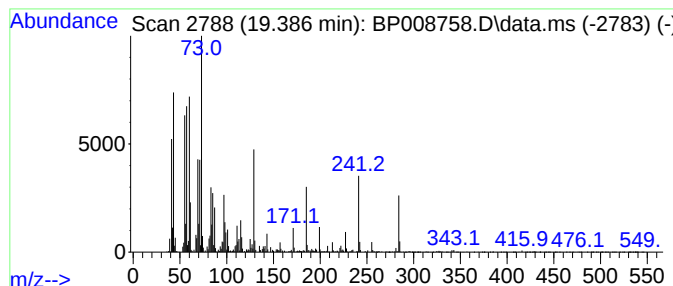
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.386	3.35 ng	511362	Chrysene-d12	21.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	38



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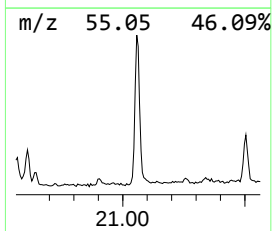
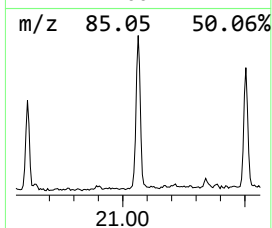
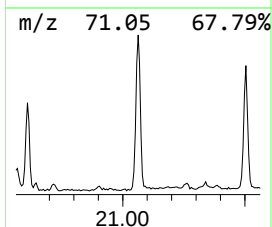
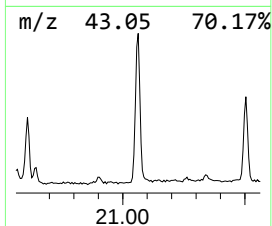
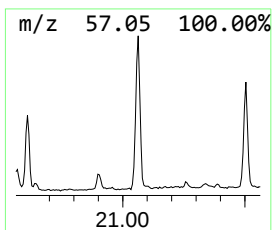
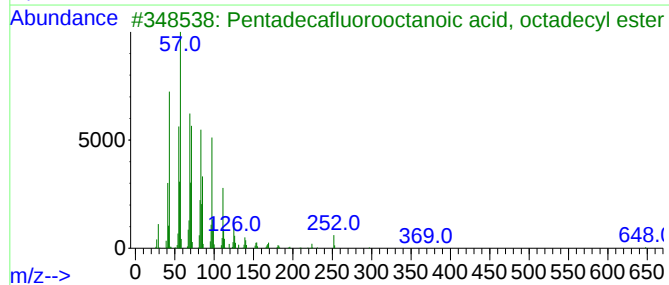
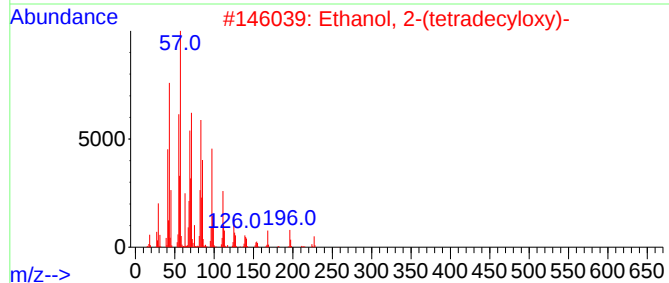
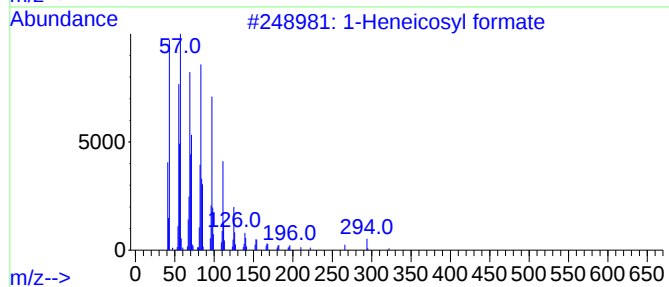
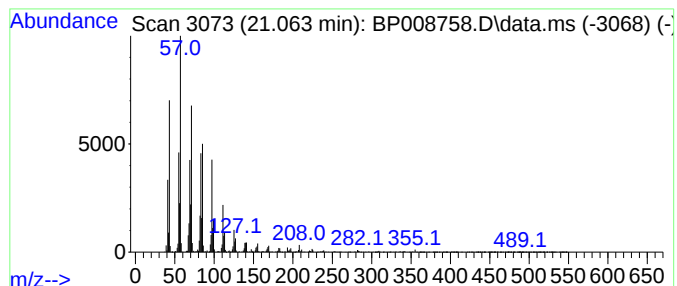
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Heneicosyl formate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.063	5.68 ng	866785	Chrysene-d12	21.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
2			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	93
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
4			Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	91
5			Carbonic acid, decyl octadecyl e...	454	C29H58O3	1000383-16-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011022\
Data File : BP008758.D
Acq On : 10 Jan 2022 19:47
Operator : CG/JU
Sample : N1054-15
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20220023-CAPE-5-MODIFIED-ELUTRIATE

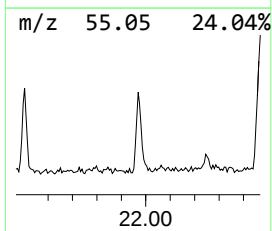
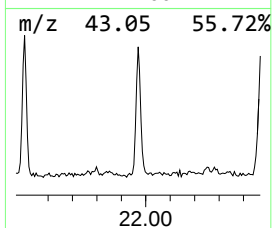
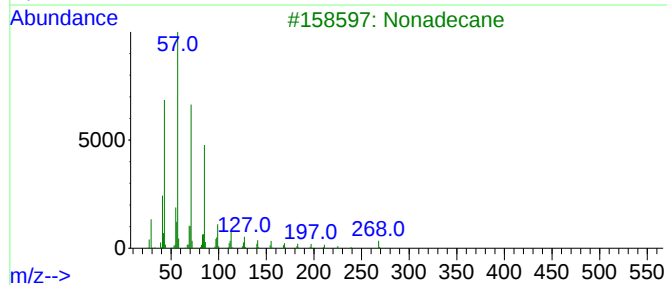
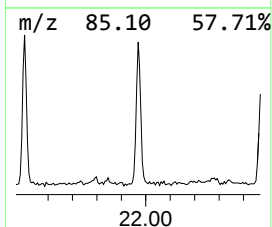
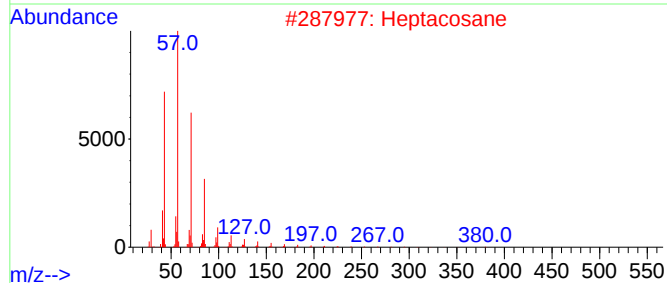
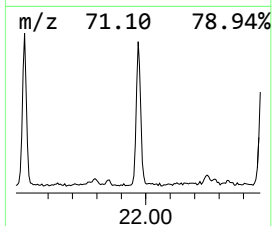
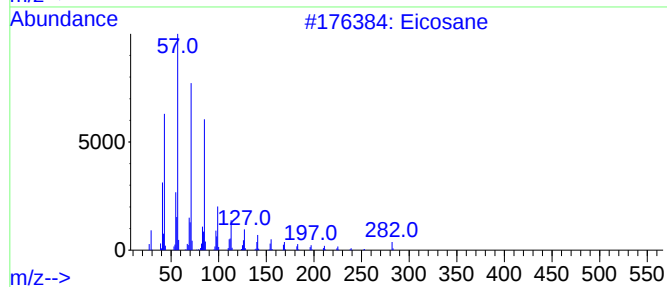
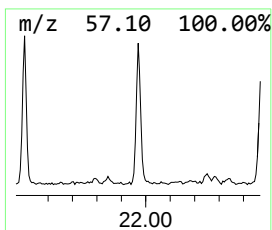
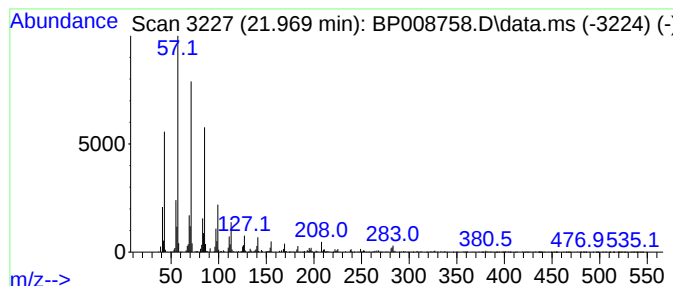
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.969	2.08 ng	317081	Chrysene-d12	21.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	98
2			Heptacosane	380	C27H56	000593-49-7	95
3			Nonadecane	268	C19H40	000629-92-5	94
4			Tritriacontane	465	C33H68	000630-05-7	93
5			Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011022\
Data File : BP008758.D
Acq On : 10 Jan 2022 19:47
Operator : CG/JU
Sample : N1054-15
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20220023-CAPE-5-MODIFIED-ELUTRIATE

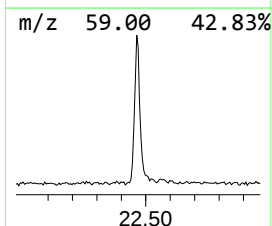
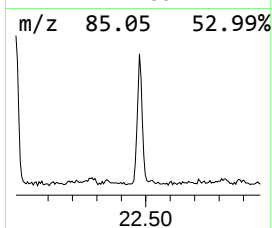
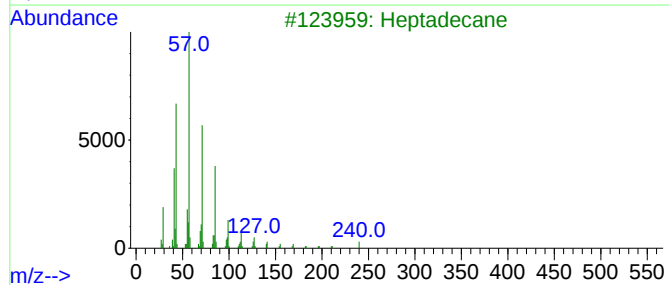
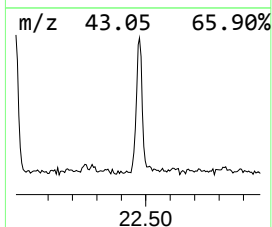
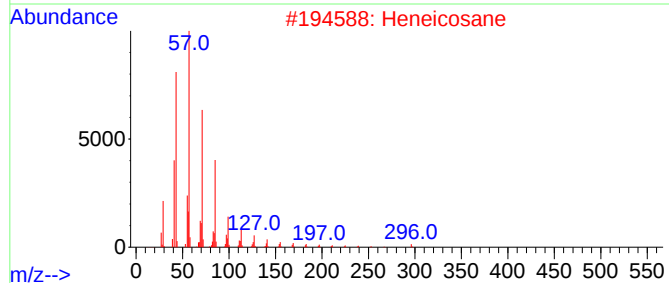
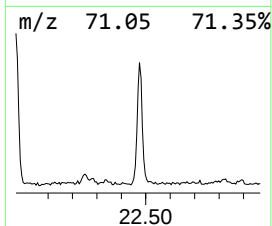
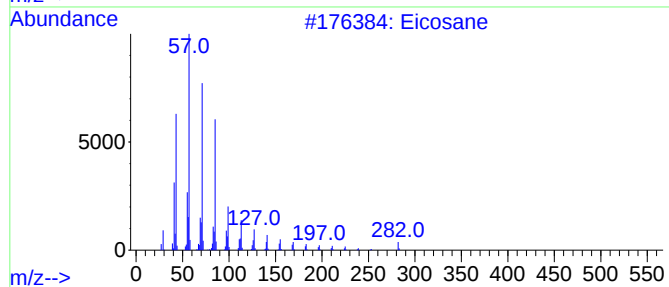
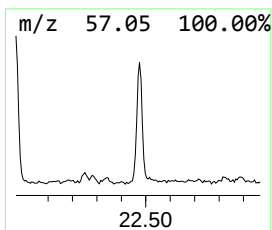
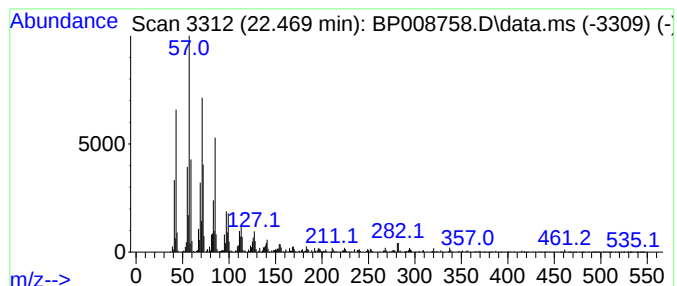
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.469	3.45 ng	525962	Chrysene-d12	21.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	95
2			Heneicosane	296	C21H44	000629-94-7	90
3			Heptadecane	240	C17H36	000629-78-7	86
4			Eicosane, 9-octyl-	394	C28H58	013475-77-9	64
5			Pentatriacontane	493	C35H72	000630-07-9	51



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011022\
Data File : BP008758.D
Acq On : 10 Jan 2022 19:47
Operator : CG/JU
Sample : N1054-15
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20220023-CAPE-5-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.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...	3.076	55.0	ng	3697460	1	7.869	1343880	20.0
2-Pentanone, 4-...	4.987	3.8	ng	252876	1	7.869	1343880	20.0
Ethanol, 2-(2-b...	10.452	5.9	ng	511181	2	10.669	1729020	20.0
n-Hexadecanoic ...	18.151	4.0	ng	513665	4	17.257	2581110	20.0
Octadecanoic acid	19.386	3.4	ng	511362	5	21.345	3052690	20.0
1-Heneicosyl fo...	21.063	5.7	ng	866785	5	21.345	3052690	20.0
Heptacosane	21.969	2.1	ng	317081	5	21.345	3052690	20.0
Heneicosane	22.469	3.5	ng	525962	5	21.345	3052690	20.0