LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121521\
Data File : BP008415.D
Acq On : 15 Dec 2021 14:07
Operator : CG/JU
Sample : M5076-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-15-C

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-BP121421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008415.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.875	316	321	335	rVB	226655	333965	14.32%	2.106%
2	5.346	395	401	420	rBV	755095	1240557	53.21%	7.822%
3	5.946	499	503	509	rVB	22633	34210	1.47%	0.216%
4	6.940	665	672	693	rBV	663799	1260699	54.07%	7.949%
5	7.740	802	808	818	rBV	213105	351790	15.09%	2.218%
6	8.904	999	1006	1024	rBV	421864	800804	34.35%	5.050%
7	10.363	1247	1254	1267	rBV2	19381	57678	2.47%	0.364%
8	10.540	1276	1284	1297	rBV	237475	441402	18.93%	2.783%
9	13.016	1697	1705	1720	rBV	1024686	1600135	68.63%	10.090%
10	14.398	1931	1940	1948	rBV	362188	580267	24.89%	3.659%
11	15.904	2187	2196	2215	rBV	701196	1282441	55.00%	8.087%
12	17.086	2393	2397	2402	rVB2	25015	33905	1.45%	0.214%
13	17.163	2403	2410	2415	rBV	438162	691196	29.65%	4.358%
14	17.204	2415	2417	2424	rVB3	38801	51081	2.19%	0.322%
15	17.292	2429	2432	2440	rVB4	12558	26411	1.13%	0.167%
16	17.839	2521	2525	2529	rVB	39973	48509	2.08%	0.306%
17	18.063	2560	2563	2572	rVB2	63730	106048	4.55%	0.669%
18	18.222	2586	2590	2594	rBV4	14359	23397	1.00%	0.148%
19	19.180	2748	2753	2761	rBV	103824	173366	7.44%	1.093%
20	19.310	2771	2775	2783	rBV5	25479	43586	1.87%	0.275%
21	19.533	2807	2813	2822	rVB	110978	171947	7.37%	1.084%
22	19.733	2841	2847	2853	rBV	1887626	2331538	100.00%	14.702%
23	20.410	2956	2962	2971	rBV	357900	434263	18.63%	2.738%
24	20.974	3055	3058	3067	rVB2	106353	168107	7.21%	1.060%
25	21.263	3102	3107	3112	rBV	677581	947442	40.64%	5.974%
26	21.380	3122	3127	3142	rBV	938039	1395515	59.85%	8.800%
27	22.492	3312	3316	3324	rVB	197496	292783	12.56%	1.846%
28	23.633	3504	3510	3520	rVB	468826	935826	40.14%	5.901%

Sum of corrected areas: 15858868

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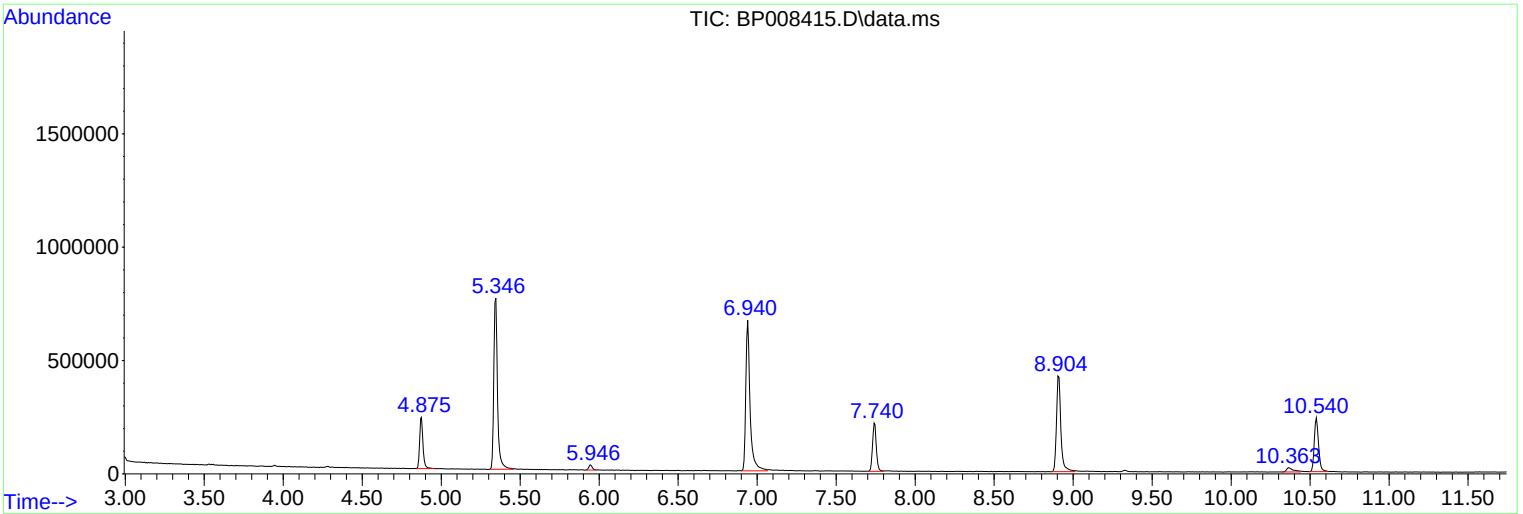
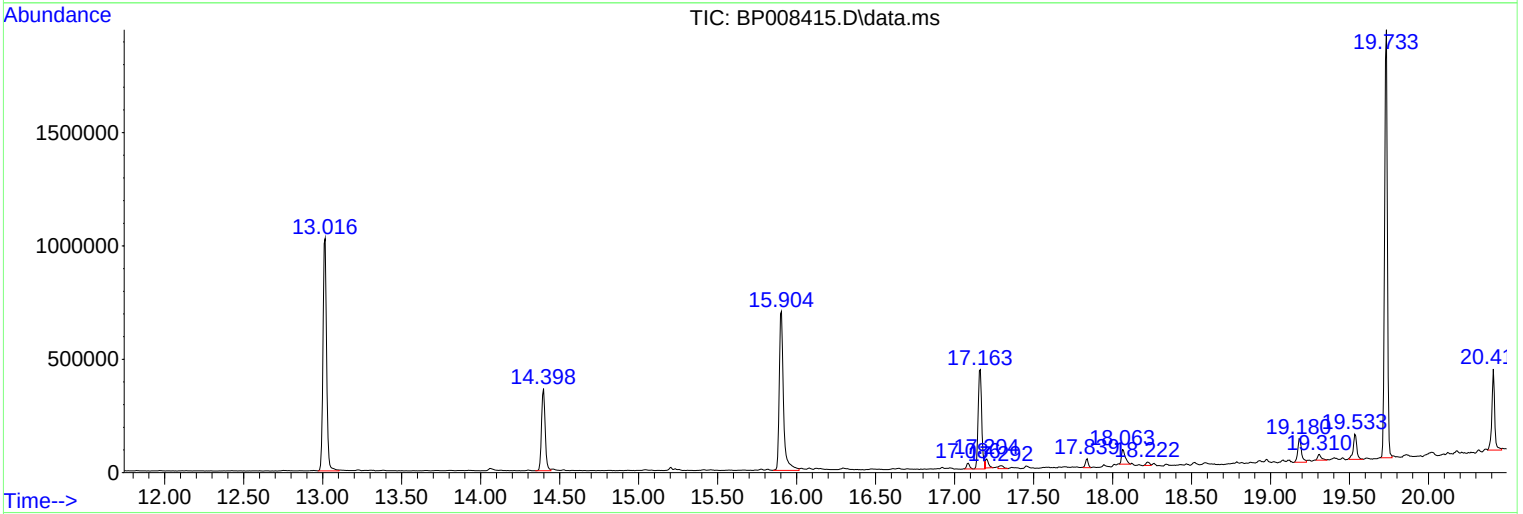
Misc :
ALS Vial : 8 Sample Multiplier: 1

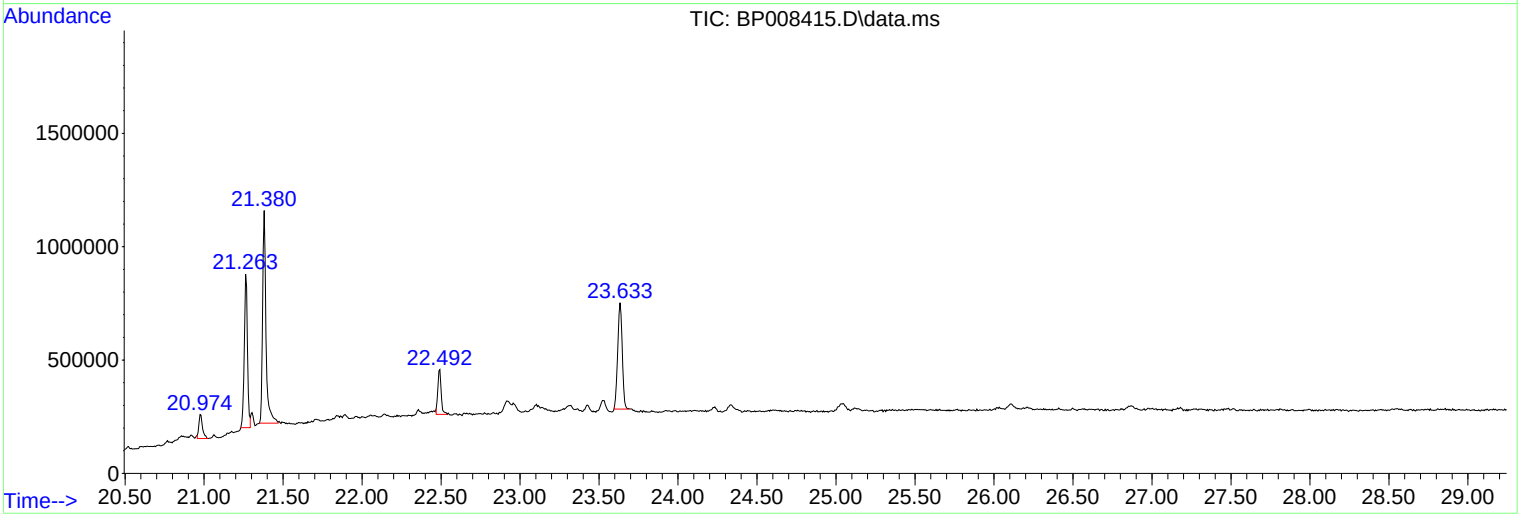
Instrument :
BNA_P
ClientSampleId :
SB-15-C

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.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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Data File : BP008415.D
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Sample : M5076-03
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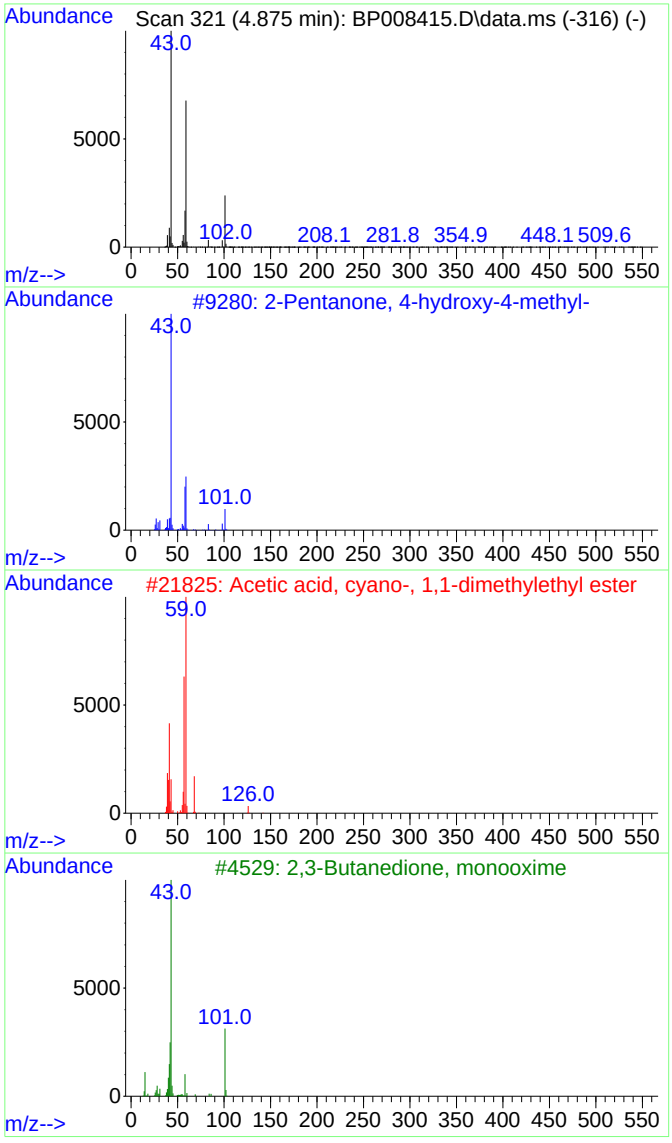
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

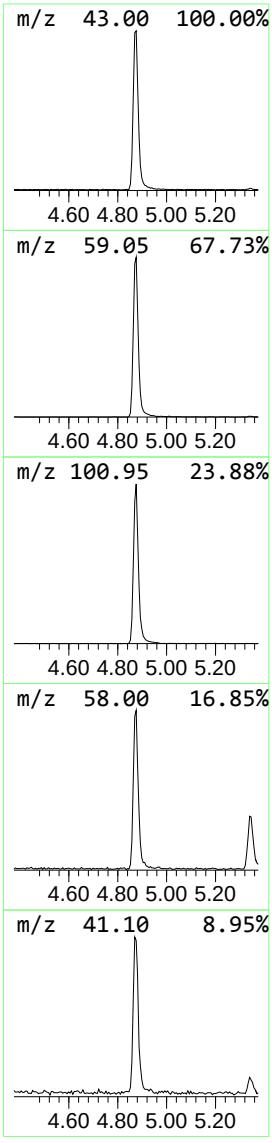
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.875	18.99 ng	333965	1,4-Dichlorobenzene-d4	7.740

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	Guanidine	59	CH5N3	000113-00-8	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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Data File : BP008415.D
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Sample : M5076-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-15-C

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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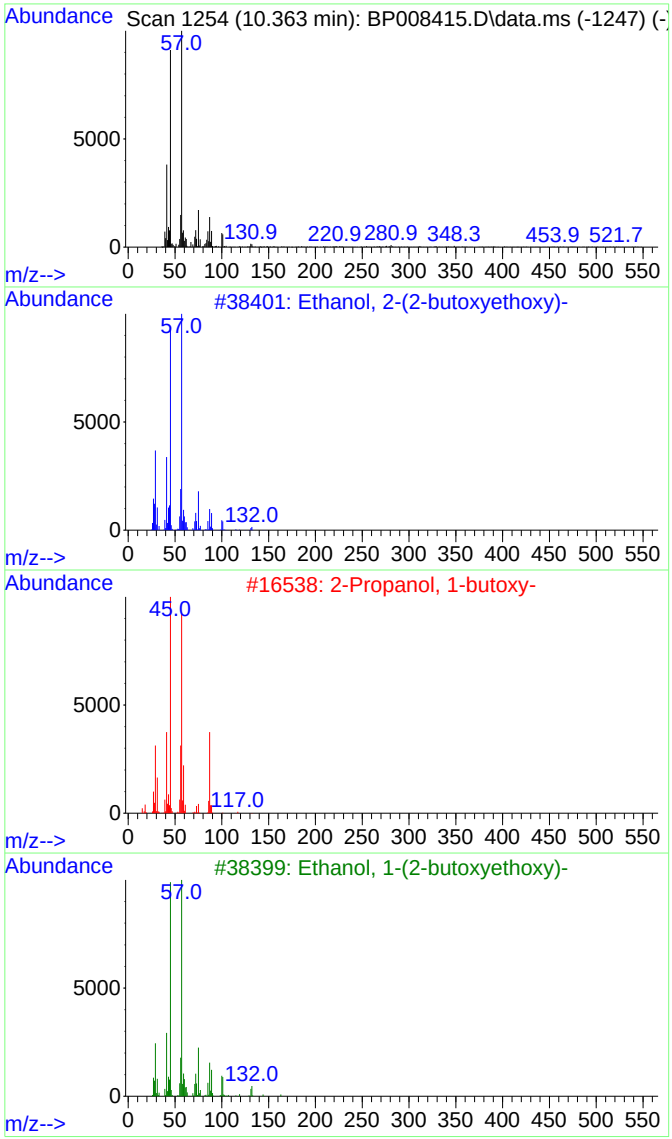
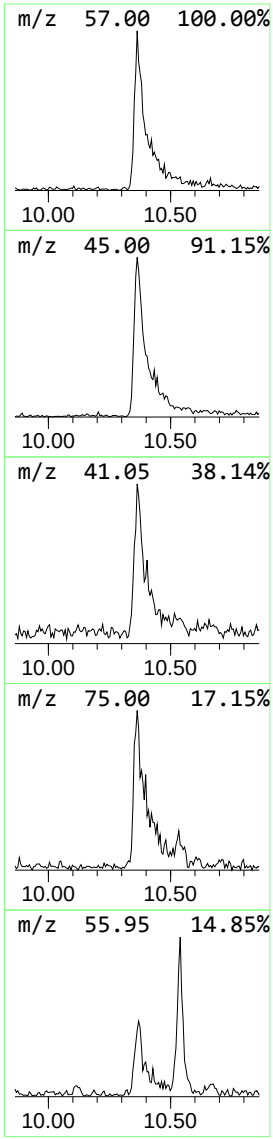
****

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.363	2.61 ng	57678	Naphthalene-d8	10.540

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	80
2	2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	72
3	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	72
4	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	64
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	59





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Acq On : 15 Dec 2021 14:07
Operator : CG/JU
Sample : M5076-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-15-C

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

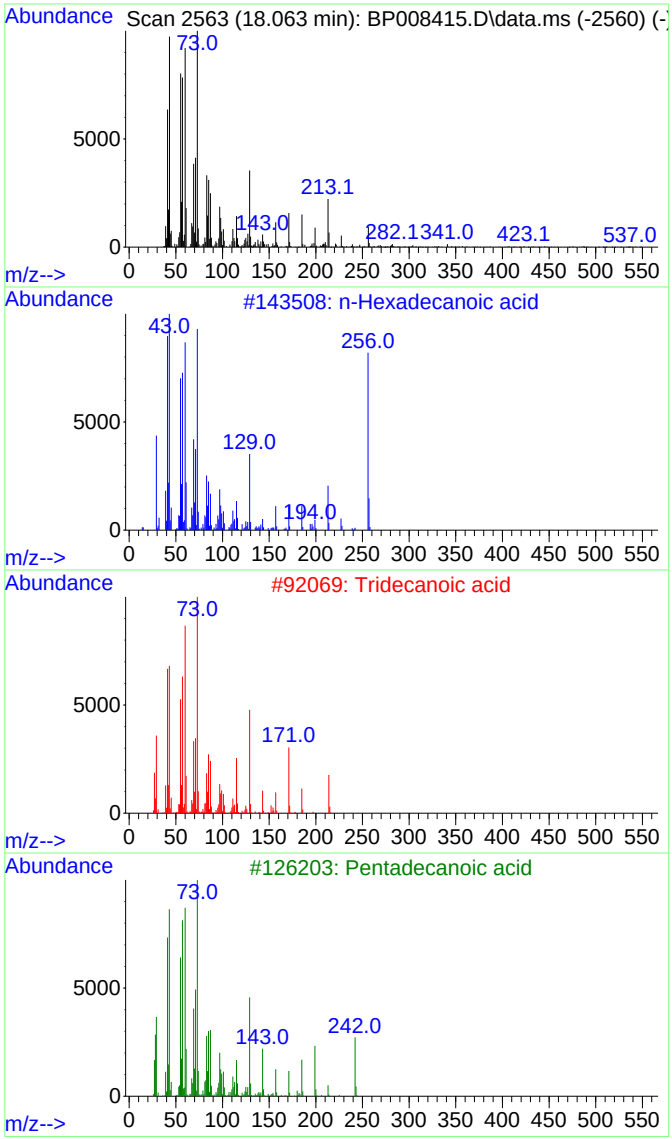
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

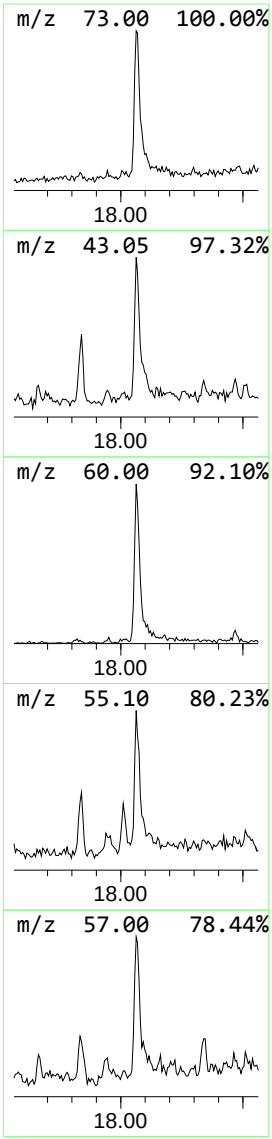
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.063	3.07 ng	106048	Phenanthrene-d10	17.163

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Nonanoic acid	158	C9H18O2	000112-05-0	55





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Data File : BP008415.D
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Sample : M5076-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-15-C

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

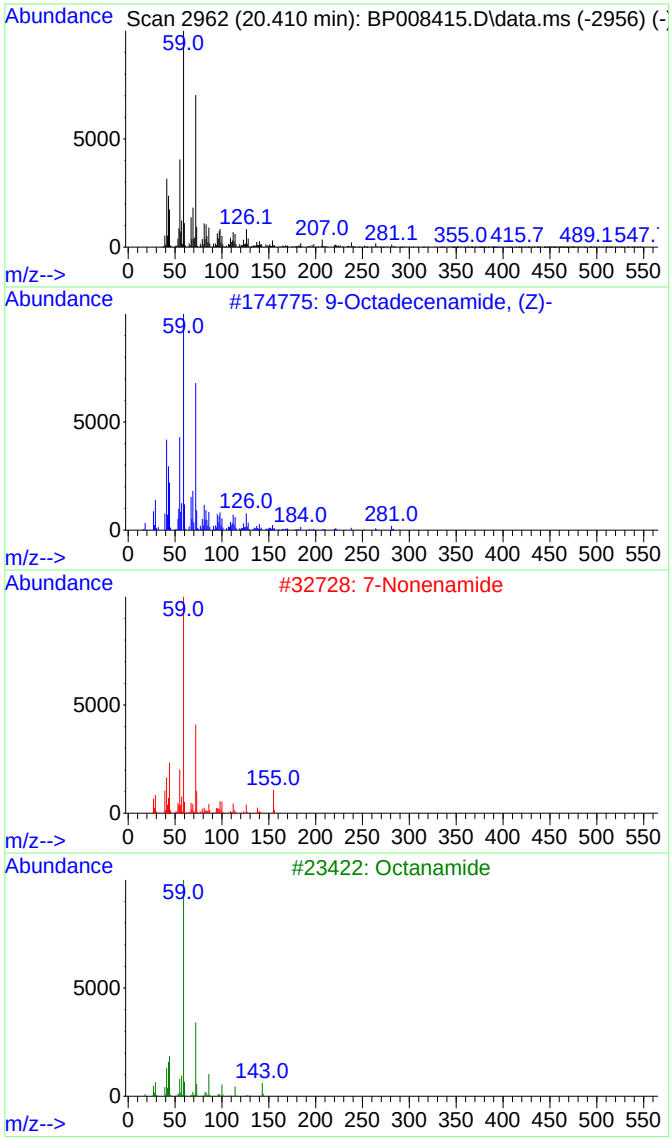
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

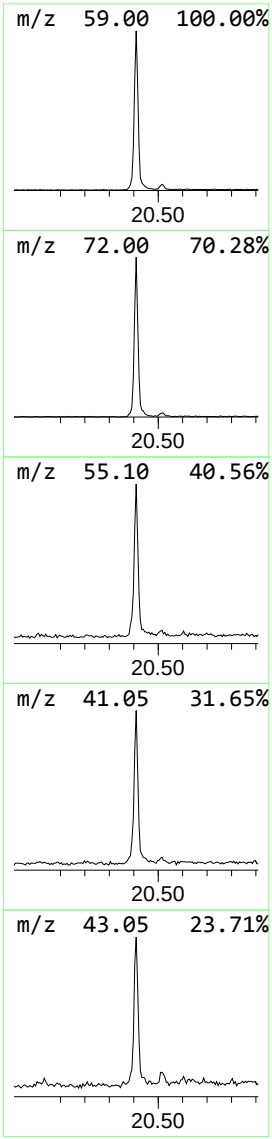
****

Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.410	9.17 ng	434263	Chrysene-d12	21.262

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2	7-Nonenamide	155	C9H17NO	090949-53-4	64
3	Octanamide	143	C8H17NO	000629-01-6	64
4	Nonanamide	157	C9H19NO	001120-07-6	59
5	N-Methyl-N-methoxycarbonylcarbam...	175	C6H9NO5	073830-21-4	58





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Data File : BP008415.D
Acq On : 15 Dec 2021 14:07
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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-15-C

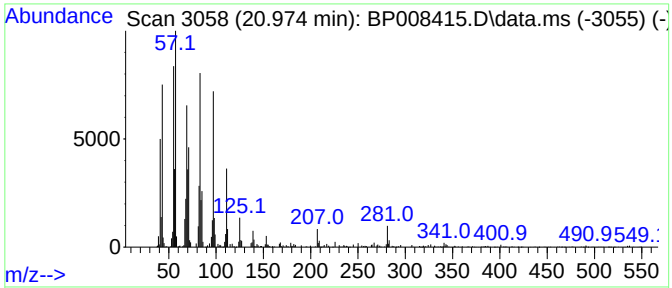
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

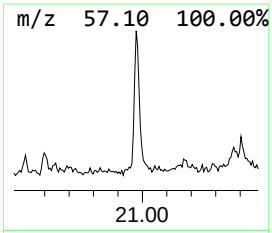
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

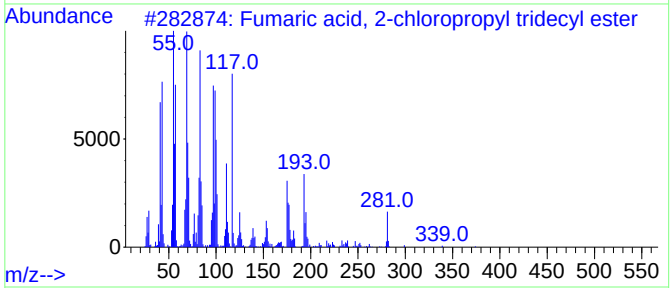
****
Peak Number 5 Fumaric acid, 2-chloropropy... Concentration Rank 5

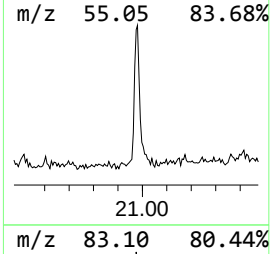
R.T.	EstConc	Area	Relative to ISTD	R.T.
20.974	3.55 ng	168107	Chrysene-d12	21.262

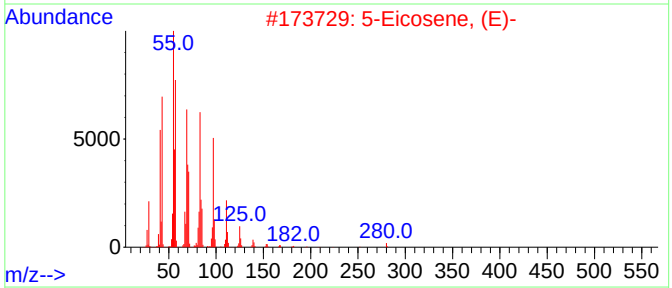
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fumaric acid, 2-chloropropyl tri...	374	C20H35ClO4	1010348-57-1	96
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	94
3	Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	93
4	1-Hexacosene	364	C26H52	018835-33-1	93
5	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	91

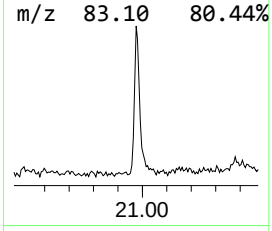


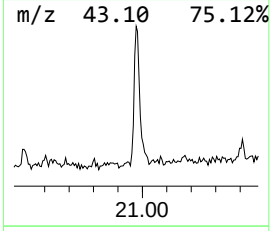


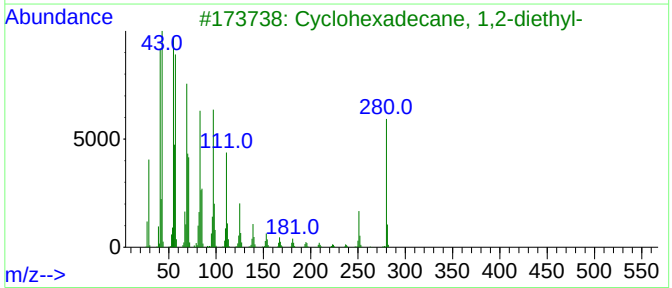


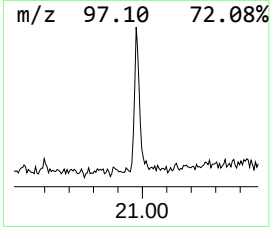












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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

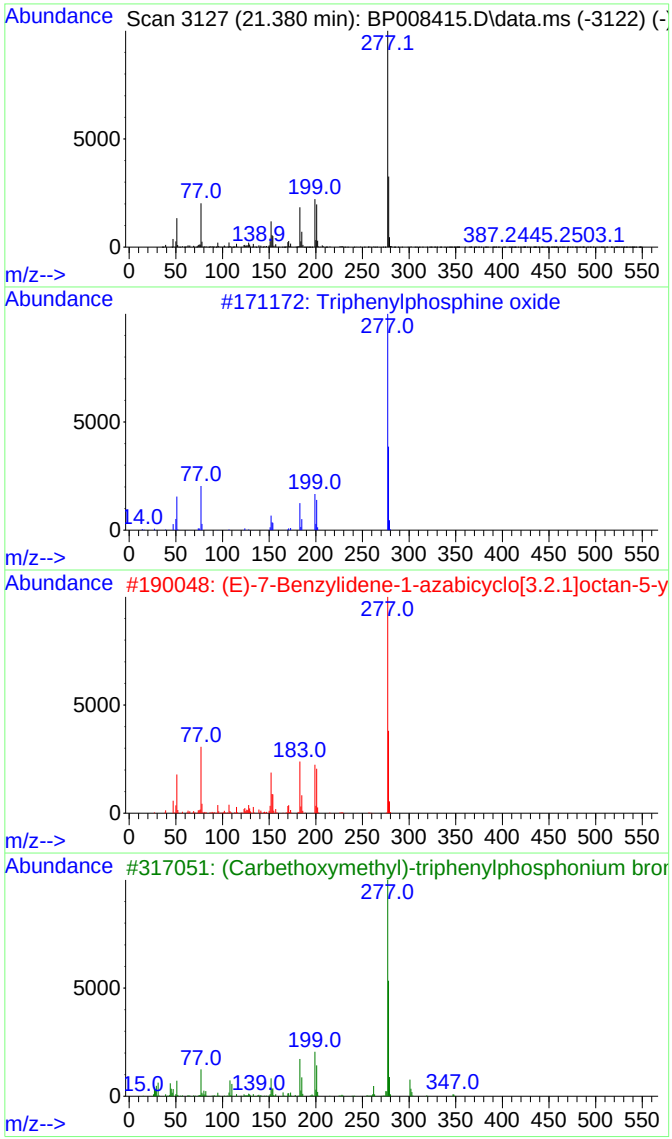
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

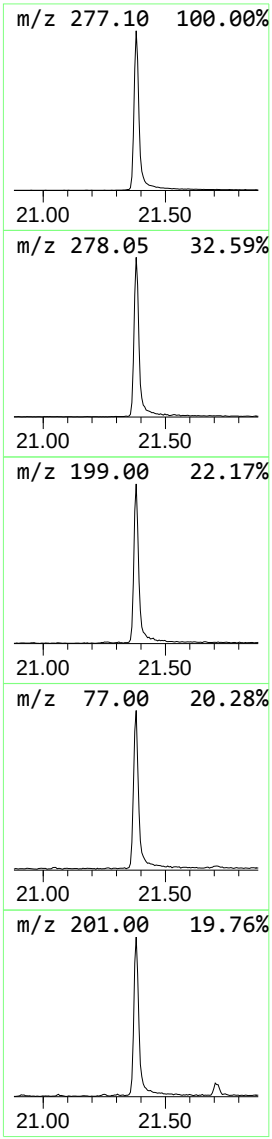
****

Peak Number 6 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.380	29.46 ng	1395520	Chrysene-d12	21.262

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	58
3	(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	50
4	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
5	3-(3,4-Dichlorophenyl)-2-thioxo-...	277	C9H5Cl2NOS2	017046-34-3	32





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

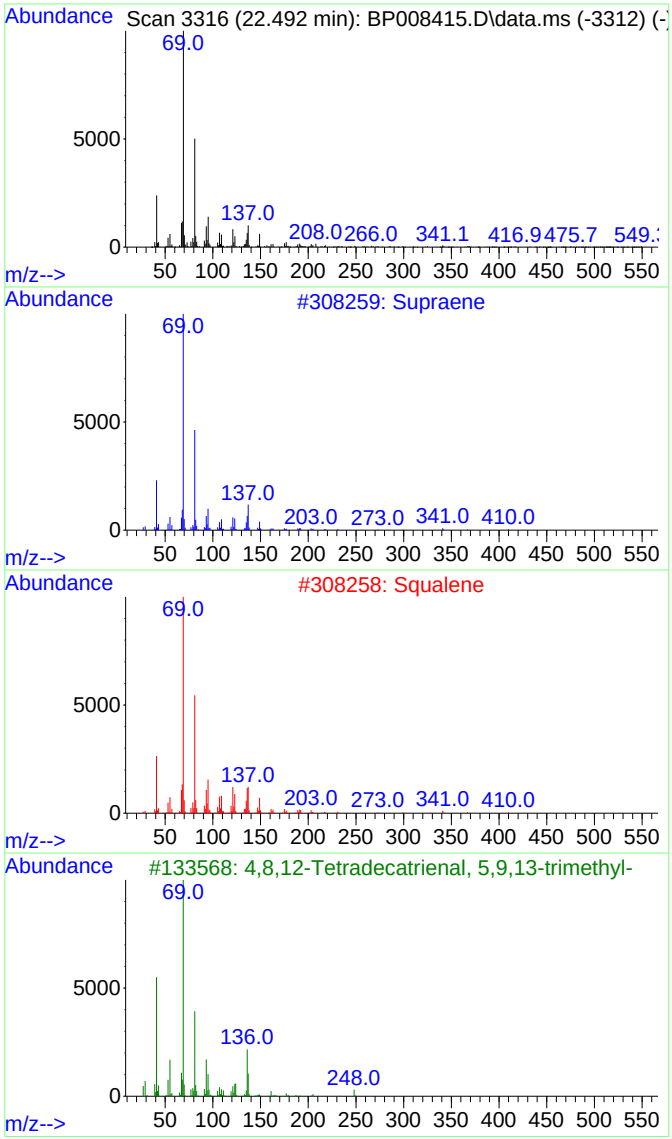
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

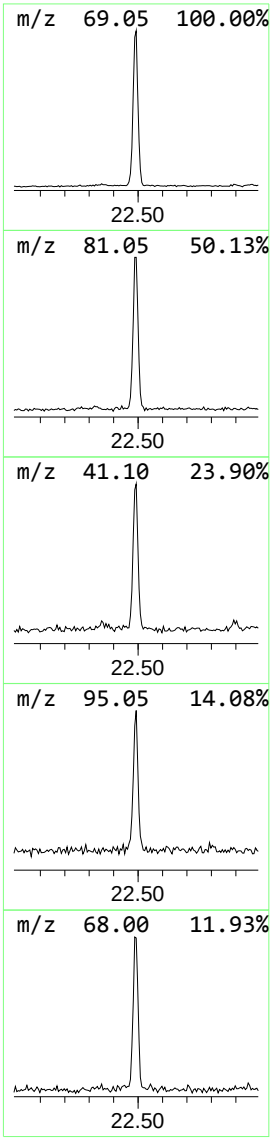
****

Peak Number 7 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.492	6.26 ng	292783	Perylene-d12	23.633

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	98
2	Squalene	410	C30H50	000111-02-4	93
3	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
5	3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	64





Tentatively Identified Compound (LSC) summary

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Data File : BP008415.D
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	4.875	19.0	ng	333965	1	7.740	351790	20.0
Ethanol, 2-(2-b...	10.363	2.6	ng	57678	2	10.540	441402	20.0
n-Hexadecanoic ...	18.063	3.1	ng	106048	4	17.163	691196	20.0
9-Octadecenamid...	20.410	9.2	ng	434263	5	21.262	947442	20.0
Fumaric acid, 2...	20.974	3.5	ng	168107	5	21.262	947442	20.0
Triphenylphosph...	21.380	29.5	ng	1395520	5	21.262	947442	20.0
Supraene	22.492	6.3	ng	292783	6	23.633	935826	20.0