LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121521\
Data File : BP008424.D
Acq On : 15 Dec 2021 19:15
Operator : CG/JU
Sample : M5017-59 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SP2-A

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: BP008424.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	330	rVB	49153	73241	4.99%	0.485%
2	5.346	395	401	418	rVB	364312	608563	41.43%	4.031%
3	6.946	667	673	682	rVV	300416	573735	39.06%	3.800%
4	7.740	798	808	815	rBV	222154	352898	24.02%	2.338%
5	7.958	841	845	852	rVB2	21587	31635	2.15%	0.210%
6	8.905	1000	1006	1025	rBV	210939	412502	28.08%	2.732%
7	9.957	1177	1185	1187	rBV9	6796	14955	1.02%	0.099%
8	10.534	1274	1283	1299	rBV	251996	463324	31.54%	3.069%
9	12.263	1571	1577	1589	rBV4	12997	36772	2.50%	0.244%
10	12.387	1591	1598	1617	rVB5	8433	30962	2.11%	0.205%
11	13.010	1697	1704	1720	rBV	571961	878738	59.82%	5.821%
12	14.063	1878	1883	1887	rBV8	7488	15474	1.05%	0.102%
13	14.116	1887	1892	1898	rVB	12222	22725	1.55%	0.151%
14	14.293	1915	1922	1927	rBV7	8252	14965	1.02%	0.099%
15	14.393	1933	1939	1946	rBV	391134	582208	39.63%	3.857%
16	14.451	1946	1949	1954	rVB5	8278	15076	1.03%	0.100%
17	14.645	1975	1982	1985	rBV9	7395	15914	1.08%	0.105%
18	14.693	1985	1990	1994	rBV3	12334	25736	1.75%	0.170%
19	14.951	2030	2034	2038	rBV2	28541	37471	2.55%	0.248%
20	15.287	2087	2091	2100	rVB4	18798	29078	1.98%	0.193%
21	15.898	2188	2195	2203	rBV	480817	728433	49.59%	4.825%
22	16.145	2228	2237	2243	rBV10	12383	32041	2.18%	0.212%
23	16.281	2256	2260	2267	rBV6	14622	21821	1.49%	0.145%
24	16.351	2268	2272	2281	rVB6	13588	25710	1.75%	0.170%
25	16.581	2306	2311	2317	rBV5	17939	35577	2.42%	0.236%
26	16.704	2325	2332	2339	rVB3	21325	49816	3.39%	0.330%
27	16.904	2362	2366	2375	rVV5	25621	55016	3.75%	0.364%
28	17.075	2391	2395	2402	rBV4	21974	41100	2.80%	0.272%
29	17.157	2402	2409	2413	rVV	521413	754271	51.35%	4.996%
30	17.204	2413	2417	2421	rVV2	115896	169752	11.56%	1.124%
31	17.251	2422	2425	2429	rVV2	31907	46264	3.15%	0.306%
32	17.292	2429	2432	2437	rVB	31634	43024	2.93%	0.285%
33	17.381	2445	2447	2453	rVB7	13490	16217	1.10%	0.107%
34	17.463	2458	2461	2465	rVB4	13390	17394	1.18%	0.115%
35	17.528	2469	2472	2475	rBV4	23318	33013	2.25%	0.219%
36	17.581	2475	2481	2485	rVB	16496	39260	2.67%	0.260%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121521\
Data File : BP008424.D
Acq On : 15 Dec 2021 19:15
Operator : CG/JU
Sample : M5017-59 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SP2-A

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

37	17.834	2521	2524	2528	rVB	27543	31550	2.15%	0.209%
38	17.945	2539	2543	2548	rBV4	23920	40733	2.77%	0.270%
39	18.004	2549	2553	2559	rBV2	61843	100783	6.86%	0.668%
40	18.063	2559	2563	2571	rVV2	203821	293273	19.96%	1.943%
41	18.163	2577	2580	2584	rVB3	29814	33774	2.30%	0.224%
42	18.345	2608	2611	2616	rBV7	14420	25603	1.74%	0.170%
43	18.569	2646	2649	2656	rVB2	23314	34483	2.35%	0.228%
44	18.975	2715	2718	2723	rVB3	55630	63525	4.32%	0.421%
45	19.181	2746	2753	2766	rBV	254814	561718	38.24%	3.721%
46	19.298	2770	2773	2781	rVV3	73342	124569	8.48%	0.825%
47	19.533	2809	2813	2816	rBV	180723	223600	15.22%	1.481%
48	19.728	2841	2846	2851	rBV	1201603	1469002	100.00%	9.731%
49	20.363	2950	2954	2958	rBV4	80237	139912	9.52%	0.927%
50	20.404	2959	2961	2968	rVB6	70910	99100	6.75%	0.656%
51	20.975	3055	3058	3066	rVB2	285225	354234	24.11%	2.346%
52	21.263	3102	3107	3111	rBV	757212	1075512	73.21%	7.124%
53	21.380	3123	3127	3143	rVB	730233	1174375	79.94%	7.779%
54	21.892	3211	3214	3222	rVB3	223307	328259	22.35%	2.174%
55	22.904	3381	3386	3391	rBV2	319877	638171	43.44%	4.227%
56	22.957	3392	3395	3404	rVB2	327700	576693	39.26%	3.820%
57	23.633	3505	3510	3517	rVB2	494071	927131	63.11%	6.141%
58	24.227	3607	3611	3619	rVB	221595	435914	29.67%	2.887%

Sum of corrected areas: 15096595

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121521\
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Operator : CG/JU
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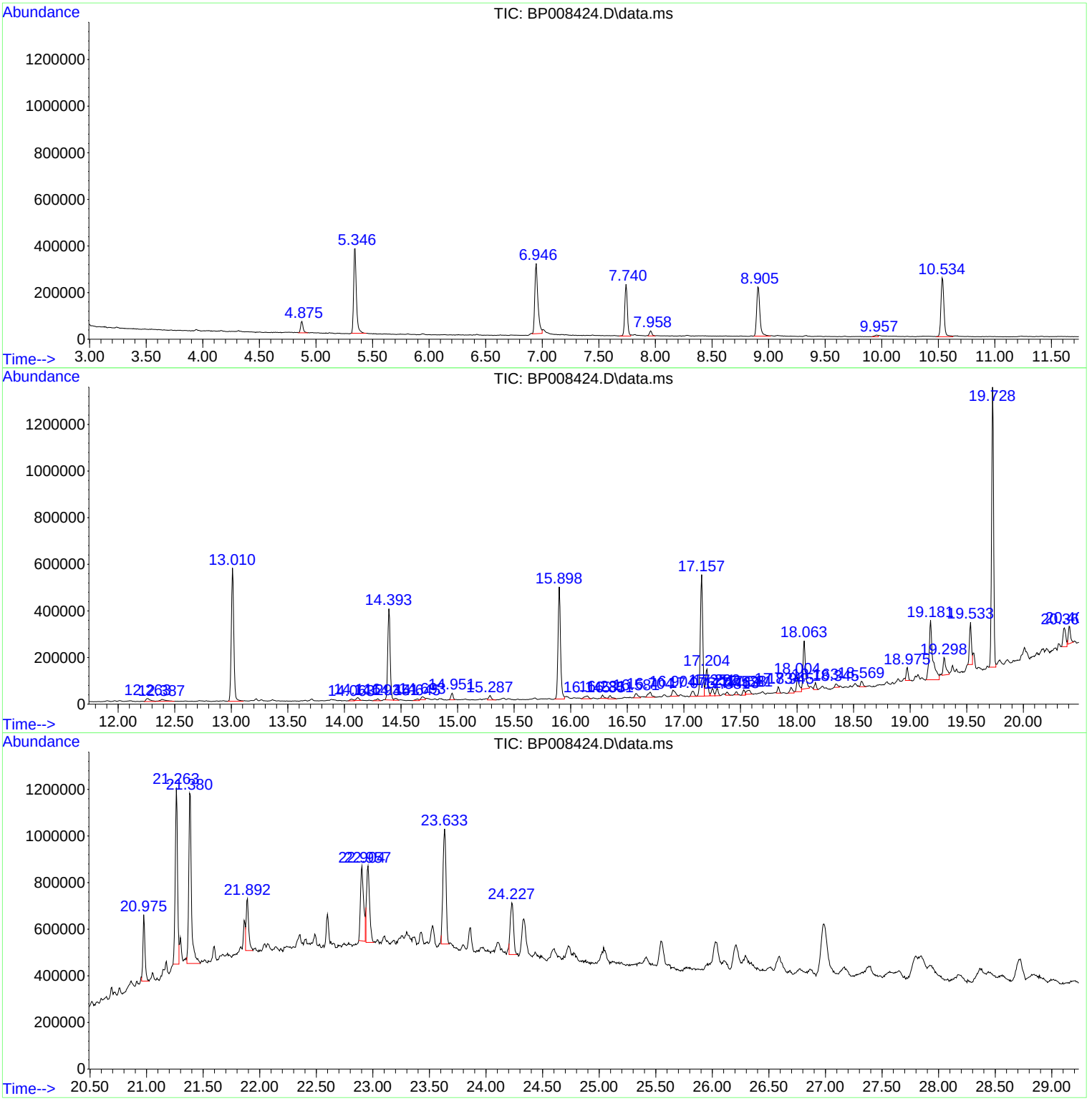
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SP2-A

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121521\
Data File : BP008424.D
Acq On : 15 Dec 2021 19:15
Operator : CG/JU
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Misc :
ALS Vial : 17 Sample Multiplier: 1

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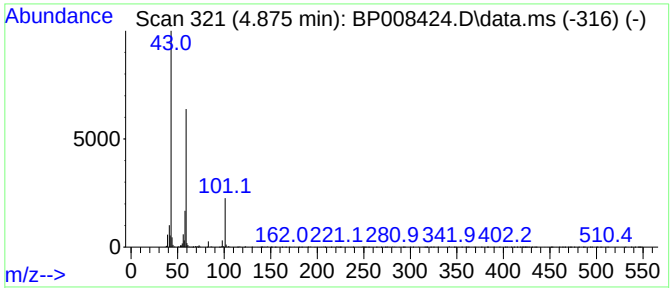
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

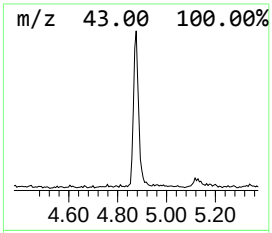
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

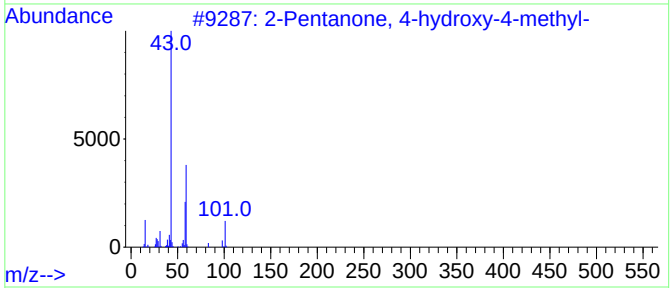
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

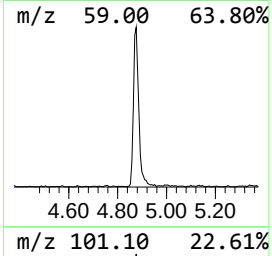
R.T.	EstConc	Area	Relative to ISTD	R.T.
4.875	4.15 ng	73241	1,4-Dichlorobenzene-d4	7.740

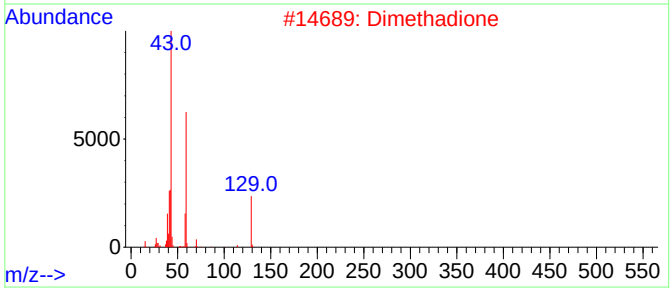
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Dimethadione	129	C5H7NO3	000695-53-4	33
3	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
4	3-Octanol	130	C8H18O	000589-98-0	28
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25

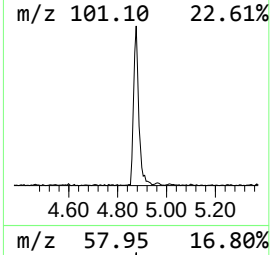


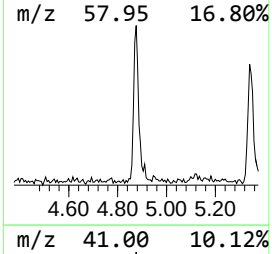


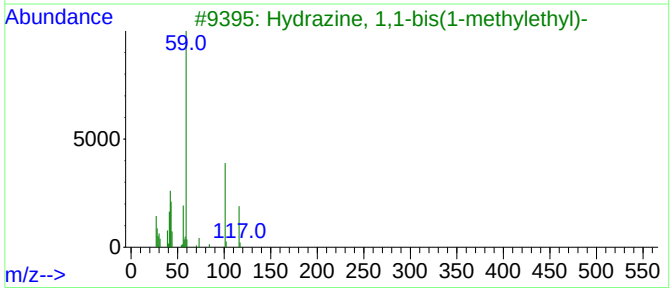


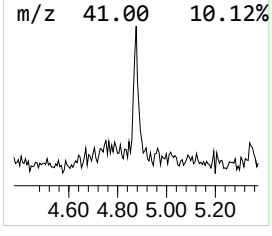












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121521\
Data File : BP008424.D
Acq On : 15 Dec 2021 19:15
Operator : CG/JU
Sample : M5017-59 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SP2-A

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

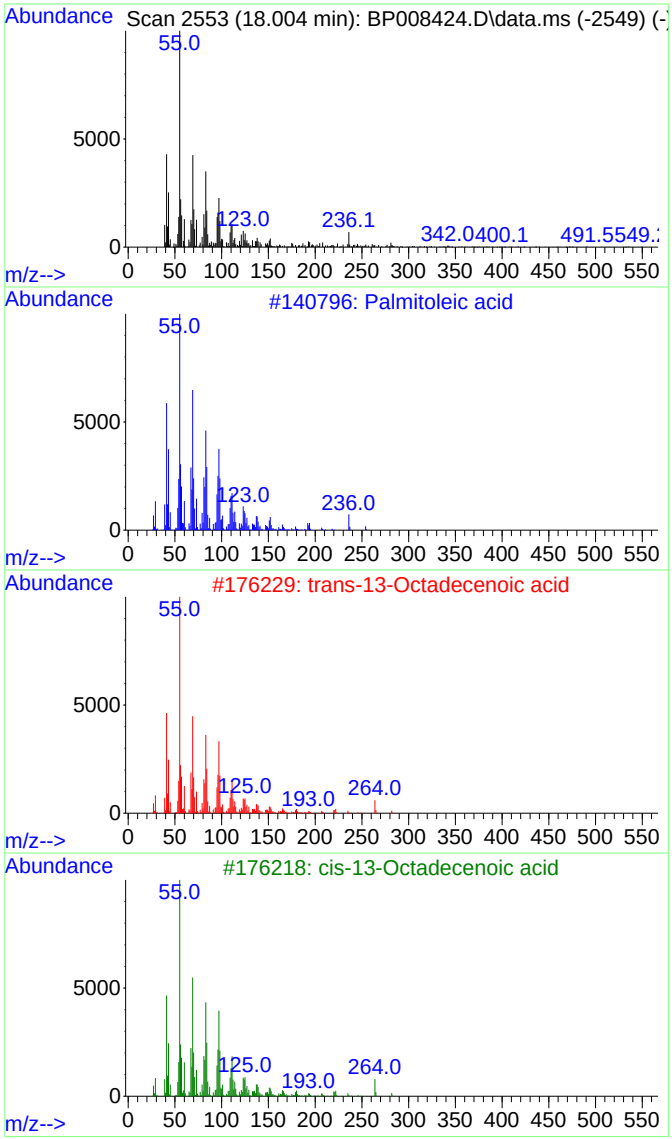
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

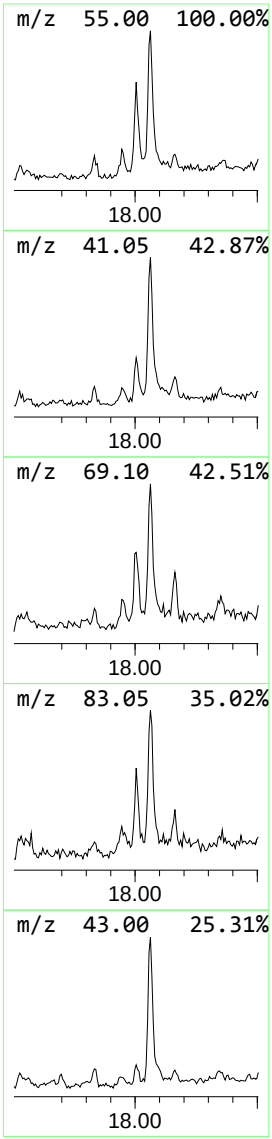
****

Peak Number 2 Palmitoleic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.004	2.67 ng	100783	Phenanthrene-d10	17.157

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Palmitoleic acid	254	C16H30O2	000373-49-9	97
2	trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	95
3	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	95
4	Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	93
5	cis-Vaccenic acid	282	C18H34O2	000506-17-2	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121521\
Data File : BP008424.D
Acq On : 15 Dec 2021 19:15
Operator : CG/JU
Sample : M5017-59 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SP2-A

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

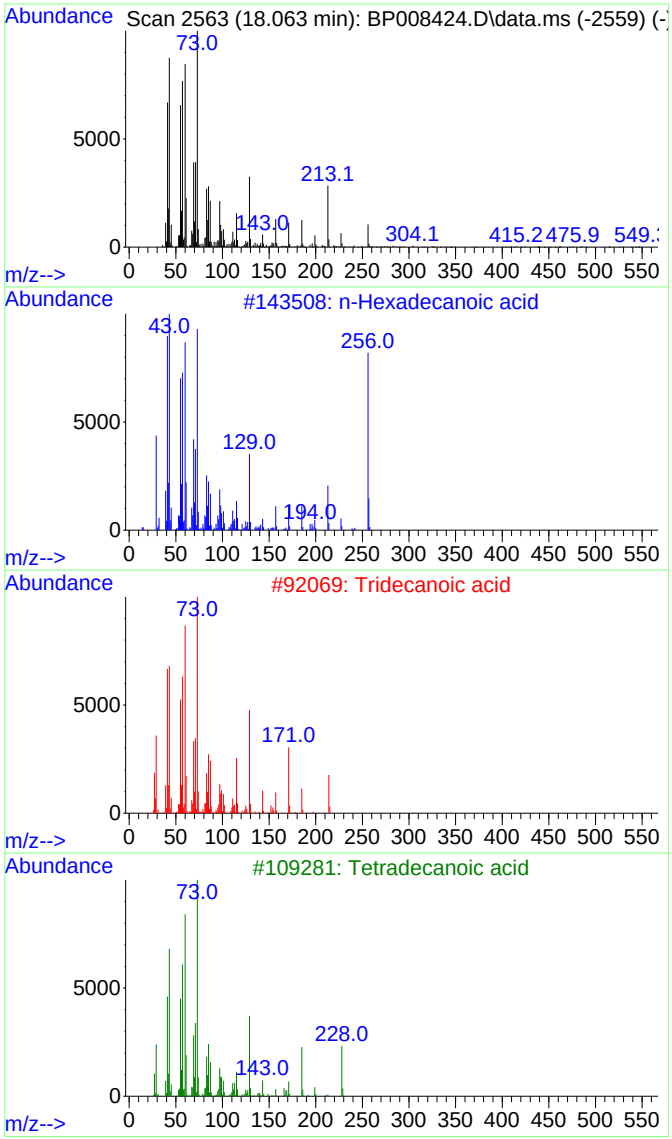
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

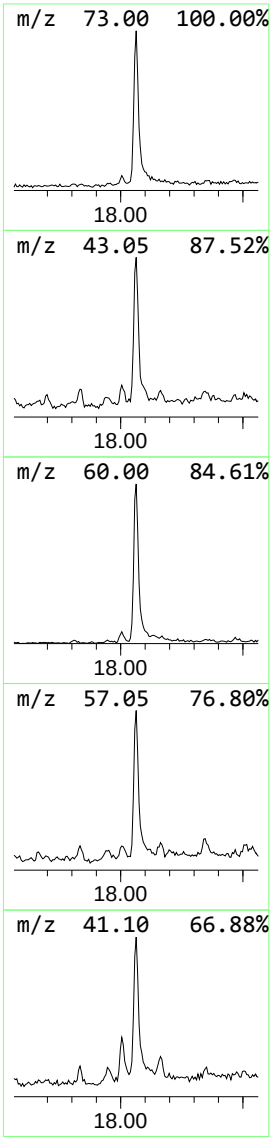
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.063	7.78 ng	293273	Phenanthrene-d10	17.157

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5	Octadecanoic acid	284	C18H36O2	000057-11-4	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121521\
Data File : BP008424.D
Acq On : 15 Dec 2021 19:15
Operator : CG/JU
Sample : M5017-59 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SP2-A

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

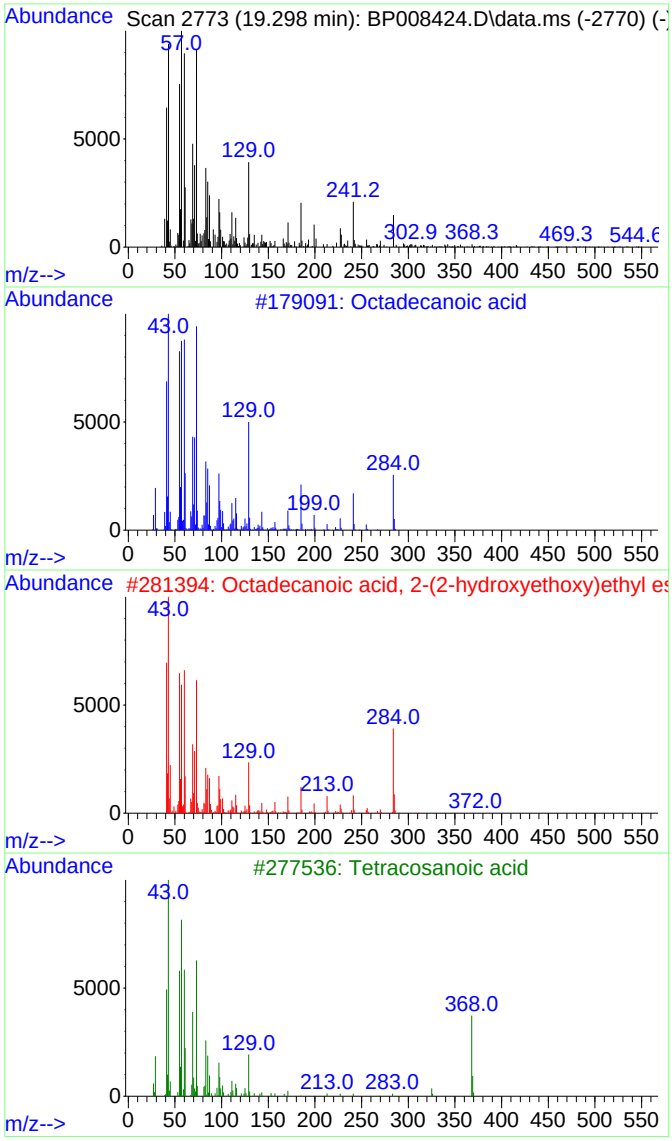
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

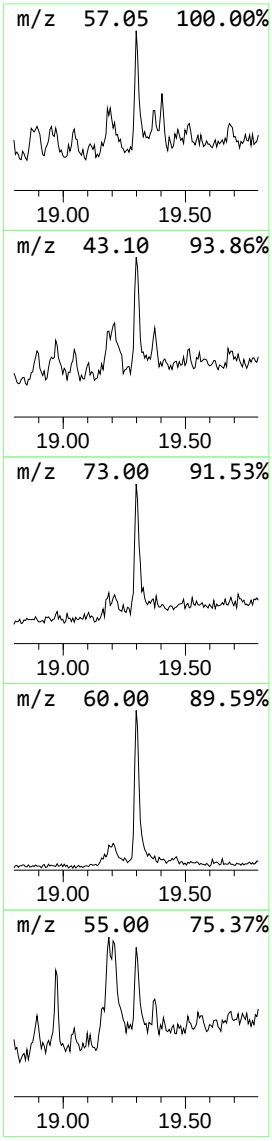
****

Peak Number 4 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.298	2.32 ng	124569	Chrysene-d12	21.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	93
3	Tetracosanoic acid	368	C24H48O2	000557-59-5	93
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121521\
Data File : BP008424.D
Acq On : 15 Dec 2021 19:15
Operator : CG/JU
Sample : M5017-59 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SP2-A

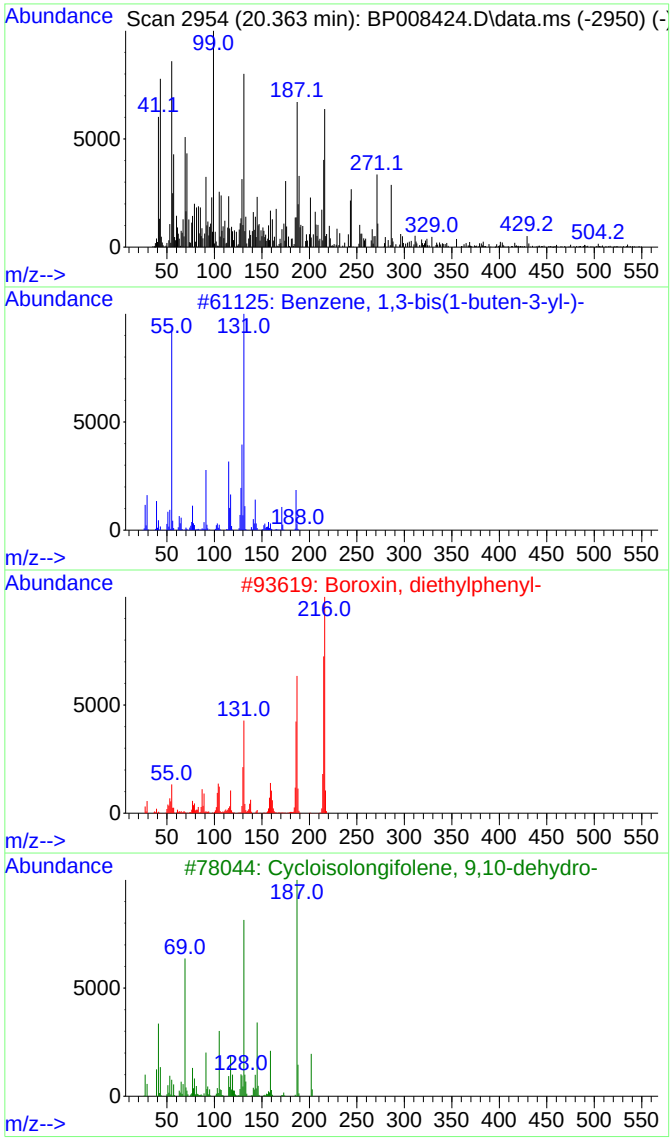
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

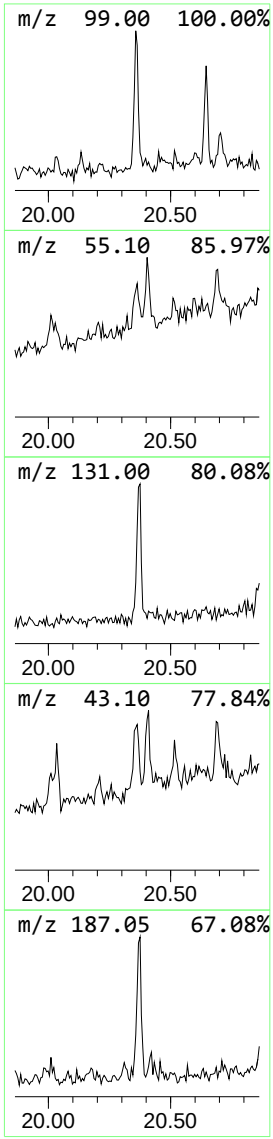
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 1,3-bis(1-buten-3-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.363	2.60 ng	139912	Chrysene-d12	21.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,3-bis(1-buten-3-yl-)-	186	C14H18	158117-62-5	53
2	Boroxin, diethylphenyl-	216	C10H15B3O3	1000151-81-1	45
3	Cycloisolongifolene, 9,10-dehydro-	202	C15H22	1000156-81-6	25
4	Cyclohexanone, 2-[(4-methoxyphen...	216	C14H16O2	005765-29-7	18
5	Esaprazole	225	C12H23N3O	064204-55-3	15





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121521\
Data File : BP008424.D
Acq On : 15 Dec 2021 19:15
Operator : CG/JU
Sample : M5017-59 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SP2-A

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

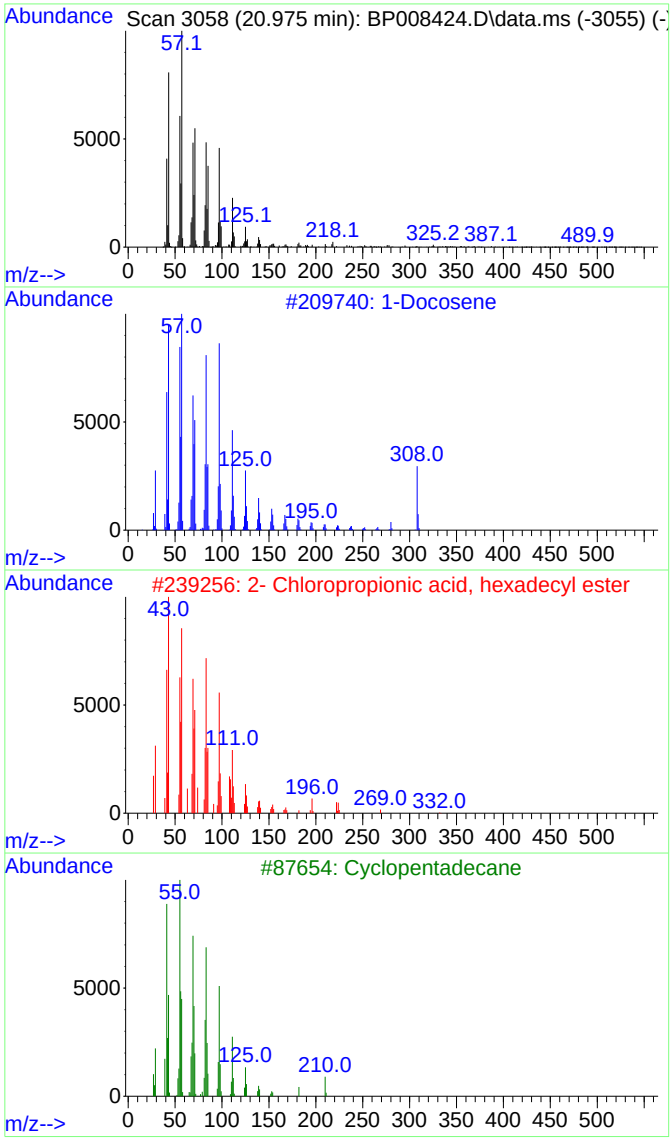
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

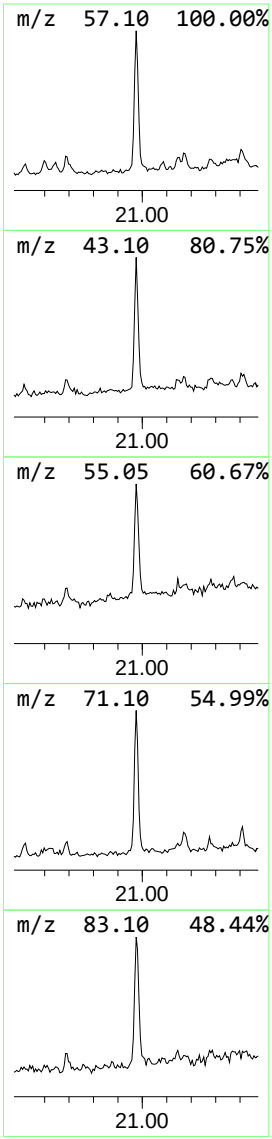
****

Peak Number 6 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.974	6.59 ng	354234	Chrysene-d12	21.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	95
2	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	93
3	Cyclopentadecane	210	C15H30	000295-48-7	92
4	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
5	17-Pentatriacontene	491	C35H70	006971-40-0	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121521\
Data File : BP008424.D
Acq On : 15 Dec 2021 19:15
Operator : CG/JU
Sample : M5017-59 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SP2-A

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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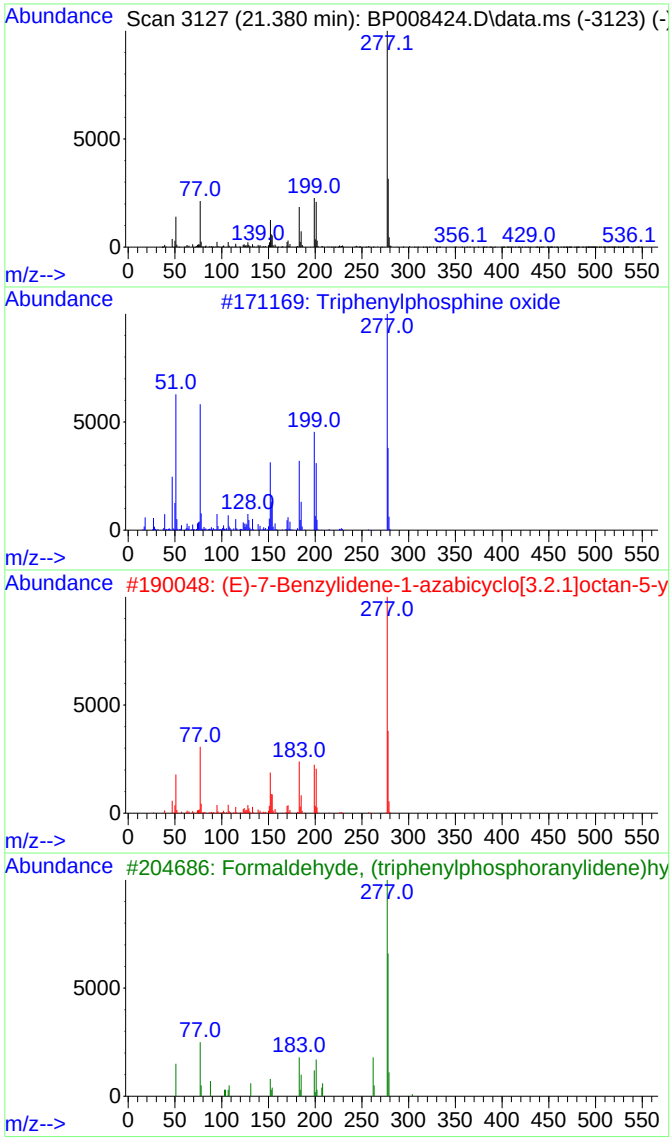
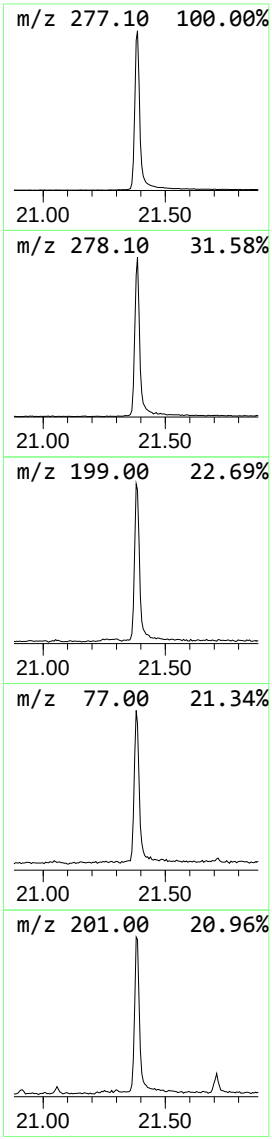
Peak Number 7 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.380	21.84 ng	1174380	Chrysene-d12	21.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	64
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	42
4	3-(3,4-Dichlorophenyl)-2-thioxo-...	277	C9H5Cl2NOS2	017046-34-3	38
5	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121521\
Data File : BP008424.D
Acq On : 15 Dec 2021 19:15
Operator : CG/JU
Sample : M5017-59 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SP2-A

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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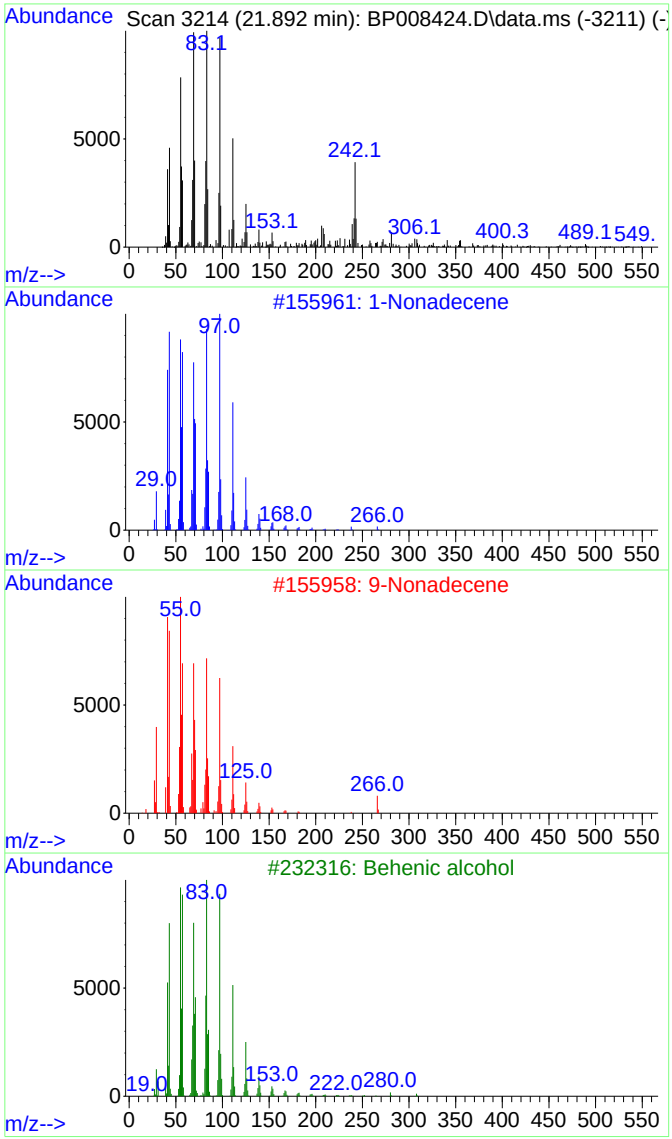
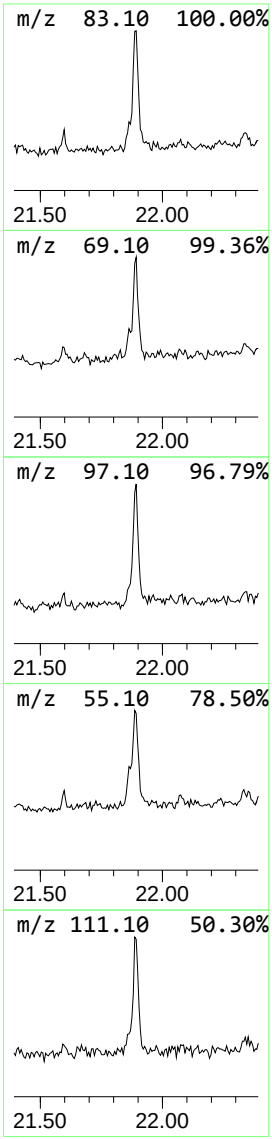
Peak Number 8 1-Nonadecene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.892	6.10 ng	328259	Chrysene-d12	21.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	92
2	9-Nonadecene	266	C19H38	031035-07-1	83
3	Behenic alcohol	326	C22H46O	000661-19-8	64
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	58
5	Fumaric acid, 2-methylallyl tetr...	366	C22H38O4	1000330-55-3	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121521\
Data File : BP008424.D
Acq On : 15 Dec 2021 19:15
Operator : CG/JU
Sample : M5017-59 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SP2-A

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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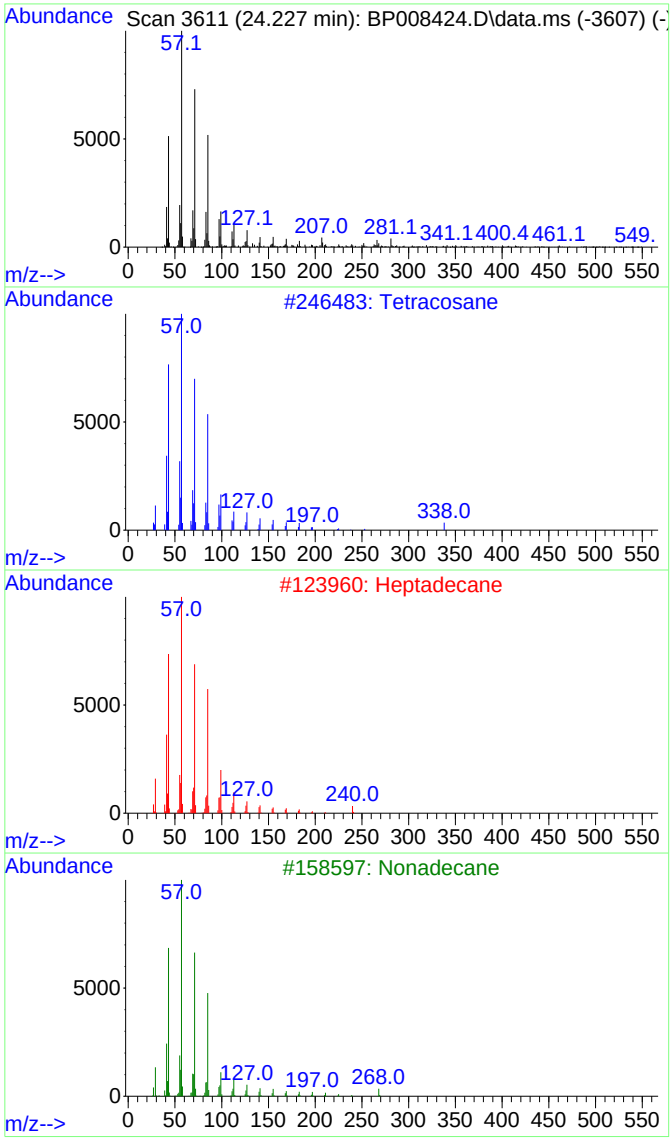
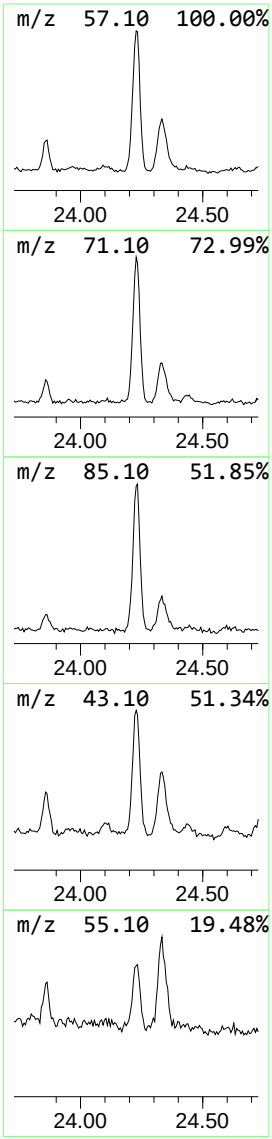
Peak Number 9 Tetracosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.227	9.40 ng	435914	Perylene-d12	23.633

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	98
2	Heptadecane	240	C17H36	000629-78-7	94
3	Nonadecane	268	C19H40	000629-92-5	93
4	Hentriacontane, 3-methyl-	451	C32H66	004981-99-1	93
5	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121521\
Data File : BP008424.D
Acq On : 15 Dec 2021 19:15
Operator : CG/JU
Sample : M5017-59 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SP2-A

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	4.875	4.2	ng	73241	1	7.740	352898	20.0
Palmitoleic acid	18.004	2.7	ng	100783	4	17.157	754271	20.0
n-Hexadecanoic ...	18.063	7.8	ng	293273	4	17.157	754271	20.0
Octadecanoic acid	19.298	2.3	ng	124569	5	21.263	1075510	20.0
Benzene, 1,3-bi...	20.363	2.6	ng	139912	5	21.263	1075510	20.0
1-Docosene	20.974	6.6	ng	354234	5	21.263	1075510	20.0
Triphenylphosph...	21.380	21.8	ng	1174380	5	21.263	1075510	20.0
1-Nonadecene	21.892	6.1	ng	328259	5	21.263	1075510	20.0
Tetracosane	24.227	9.4	ng	435914	6	23.633	927131	20.0