LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP112719\
Data File : BP001099.D
Acq On : 28 Nov 2019 00:36
Operator : JU
Sample : K6008-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : CALVTANK-1-20191121

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\8270-BP112719.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.964	141	149	161	rBV	52873	108247	1.58%	0.185%
2	4.064	331	336	347	rVB2	28819	74384	1.09%	0.127%
3	5.640	596	604	620	rBV	410030	655196	9.59%	1.117%
4	6.234	698	705	717	rVB	2730591	3612261	52.89%	6.158%
5	7.769	960	966	974	rBV	2145733	2717205	39.79%	4.632%
6	7.963	992	999	1004	rBV	4146495	5326241	77.99%	9.080%
7	8.328	1055	1061	1067	rBV	999806	1163613	17.04%	1.984%
8	8.569	1096	1102	1106	rBV	3271335	3875117	56.74%	6.606%
9	9.210	1204	1211	1215	rBV	2840945	3588664	52.55%	6.118%
10	10.363	1401	1407	1412	rBV	1309546	1536455	22.50%	2.619%
11	12.146	1703	1710	1714	rBV	5301273	6517556	95.43%	11.111%
12	12.810	1818	1823	1828	rBV	785545	878390	12.86%	1.497%
13	13.228	1888	1894	1899	rBV	1571779	1933894	28.32%	3.297%
14	13.381	1904	1920	1929	rBV	2061458	5818255	85.19%	9.919%
15	13.910	2005	2010	2016	rVB	89750	100283	1.47%	0.171%
16	14.522	2107	2114	2128	rBV	3487744	4665833	68.32%	7.954%
17	15.622	2296	2301	2306	rBV	1732979	1989625	29.13%	3.392%
18	16.516	2448	2453	2475	rBV	775528	1129489	16.54%	1.926%
19	17.598	2634	2637	2653	rBV	297611	448767	6.57%	0.765%
20	17.910	2684	2690	2694	rBV	5797022	6829491	100.00%	11.643%
21	18.728	2825	2829	2832	rBV	83683	82916	1.21%	0.141%
22	19.157	2897	2902	2904	rBV	111754	157844	2.31%	0.269%
23	19.198	2904	2909	2916	rVV7	140725	489345	7.17%	0.834%
24	19.263	2916	2920	2926	rVB	1435789	1689742	24.74%	2.881%
25	19.563	2967	2971	2978	rVB	157827	168245	2.46%	0.287%
26	19.951	3033	3037	3042	rBV	185251	201732	2.95%	0.344%
27	20.327	3097	3101	3106	rBV	224183	248642	3.64%	0.424%
28	20.727	3164	3169	3178	rVB	212861	293582	4.30%	0.500%
29	21.045	3216	3223	3233	rVB	1071583	1532680	22.44%	2.613%
30	21.169	3239	3244	3250	rBV	185272	266023	3.90%	0.454%
31	21.669	3323	3329	3341	rBV	138211	242875	3.56%	0.414%
32	22.245	3421	3427	3435	rBV2	69571	139135	2.04%	0.237%
33	22.527	3468	3475	3488	rVB4	82576	177119	2.59%	0.302%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP112719\
Data File : BP001099.D
Acq On : 28 Nov 2019 00:36
Operator : JU
Sample : K6008-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : CALVTANK-1-20191121

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\8270-BP112719.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

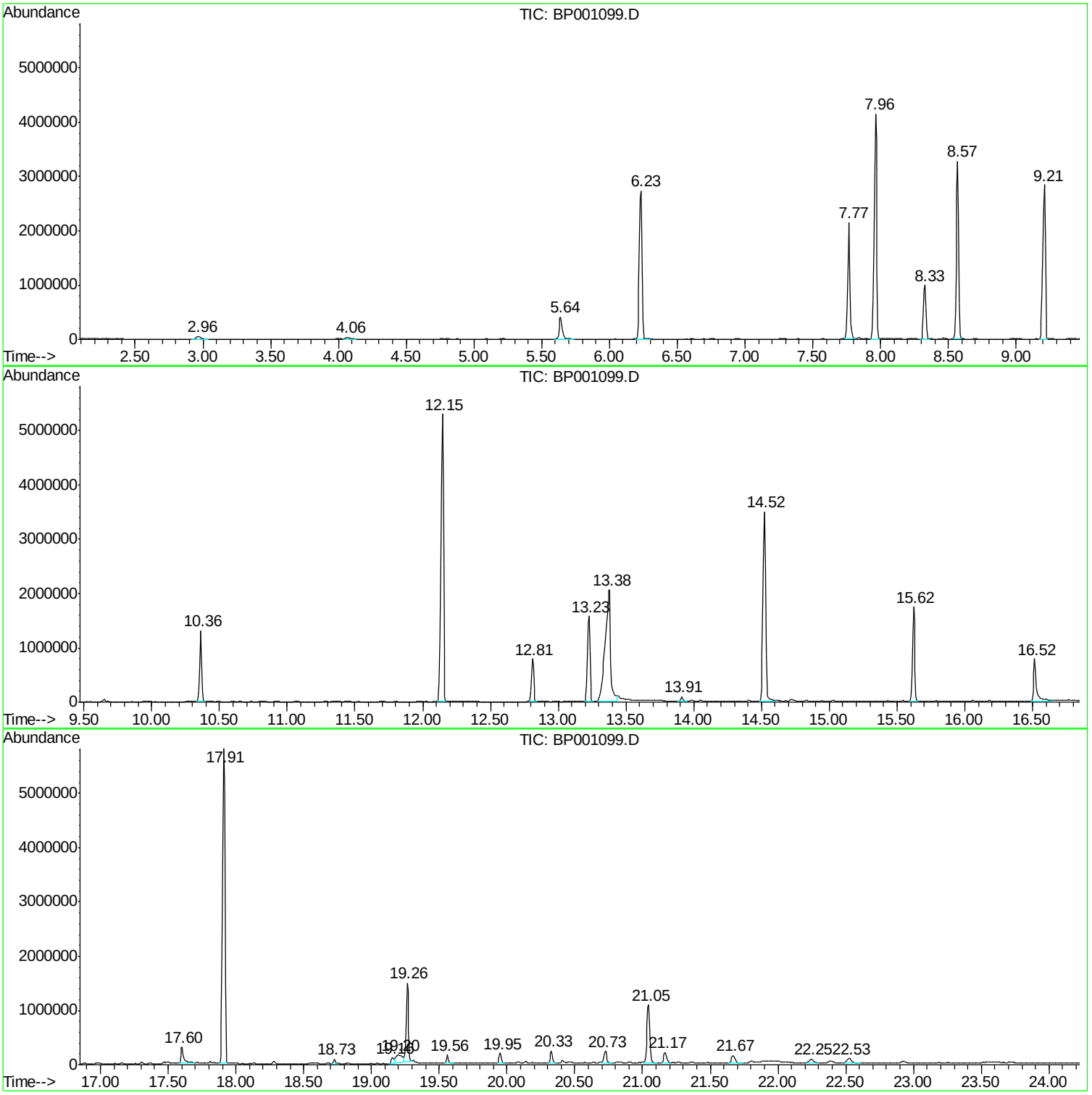
Sum of corrected areas: 58658846

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP112719\
Data File : BP001099.D
Acq On : 28 Nov 2019 00:36
Operator : JU
Sample : K6008-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : CALVTANK-1-20191121

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP112719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP112719\
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TIC Library : C:\DATABASE\NIST11.L
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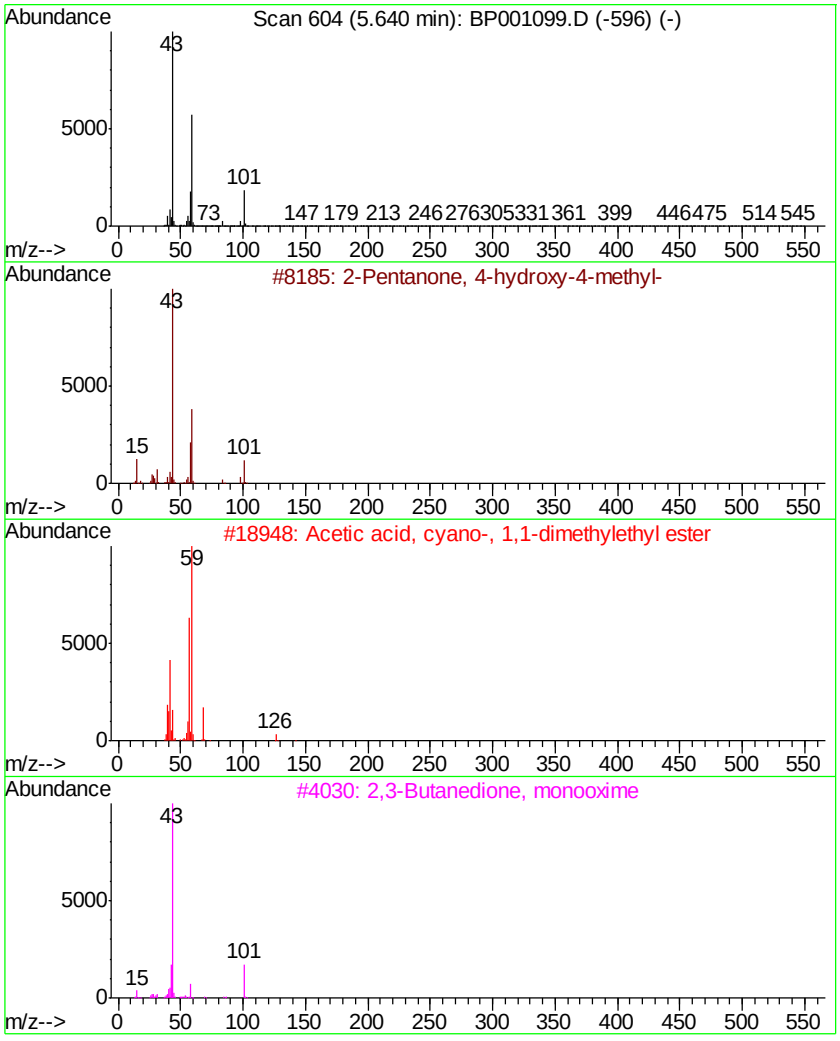
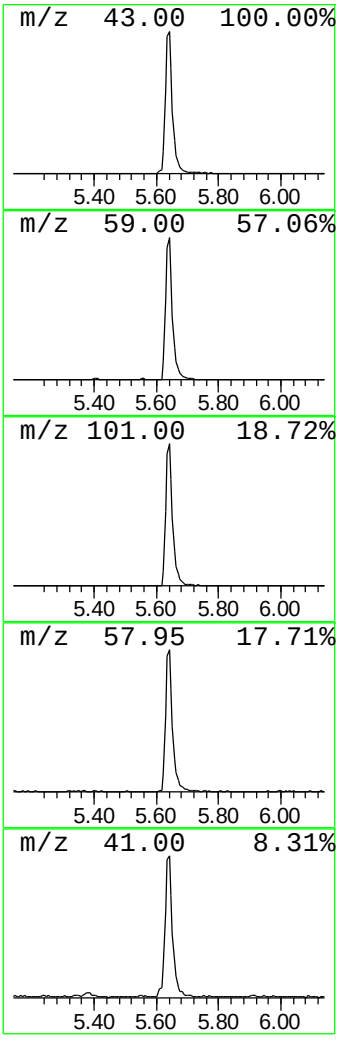
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.64	11.26 ng	655196	1,4-Dichlorobenzene-d4	8.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP112719\
Data File : BP001099.D
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Operator : JU
Sample : K6008-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : CALVTANK-1-20191121

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP112719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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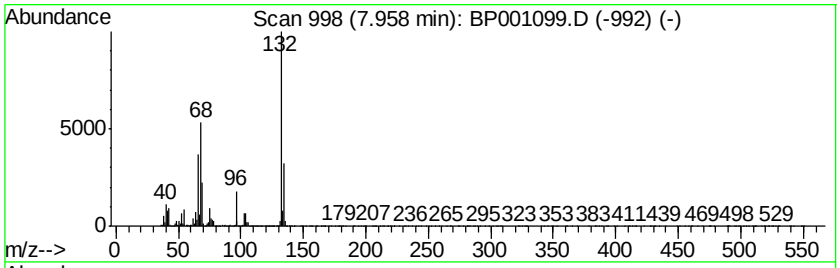
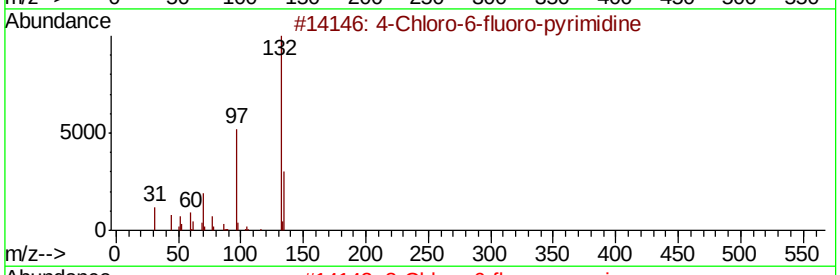
****

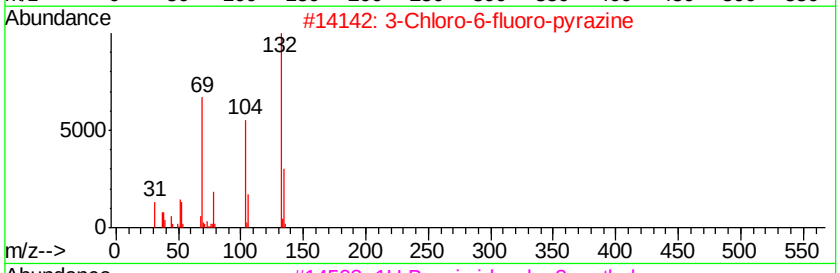
Peak Number 2 unknown7.96 Concentration Rank 1

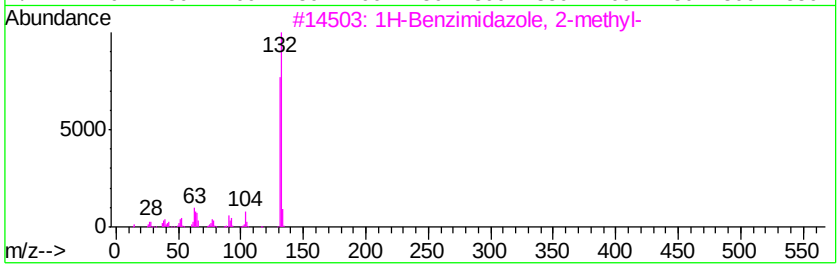
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.96	91.55 ng	5326240	1,4-Dichlorobenzene-d4	8.33

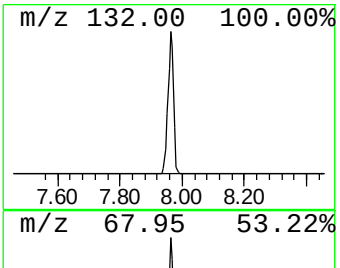
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	5-Aminoindole	132	C8H8N2	005192-03-0	22
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12

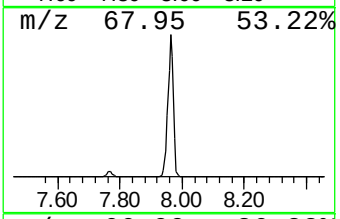


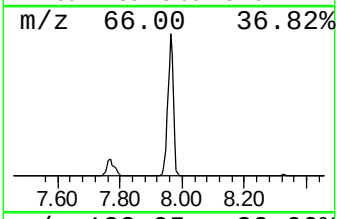


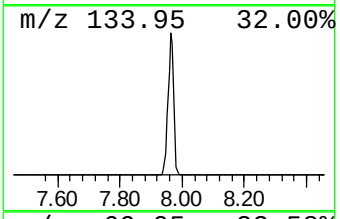


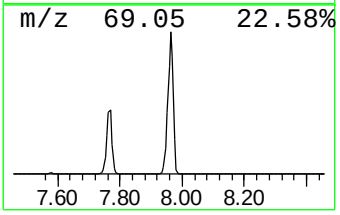












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Data File : BP001099.D
Acq On : 28 Nov 2019 00:36
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Sample : K6008-01
Misc :
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Instrument : BNA_P
ClientSampleId : CALVTANK-1-20191121

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP112719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

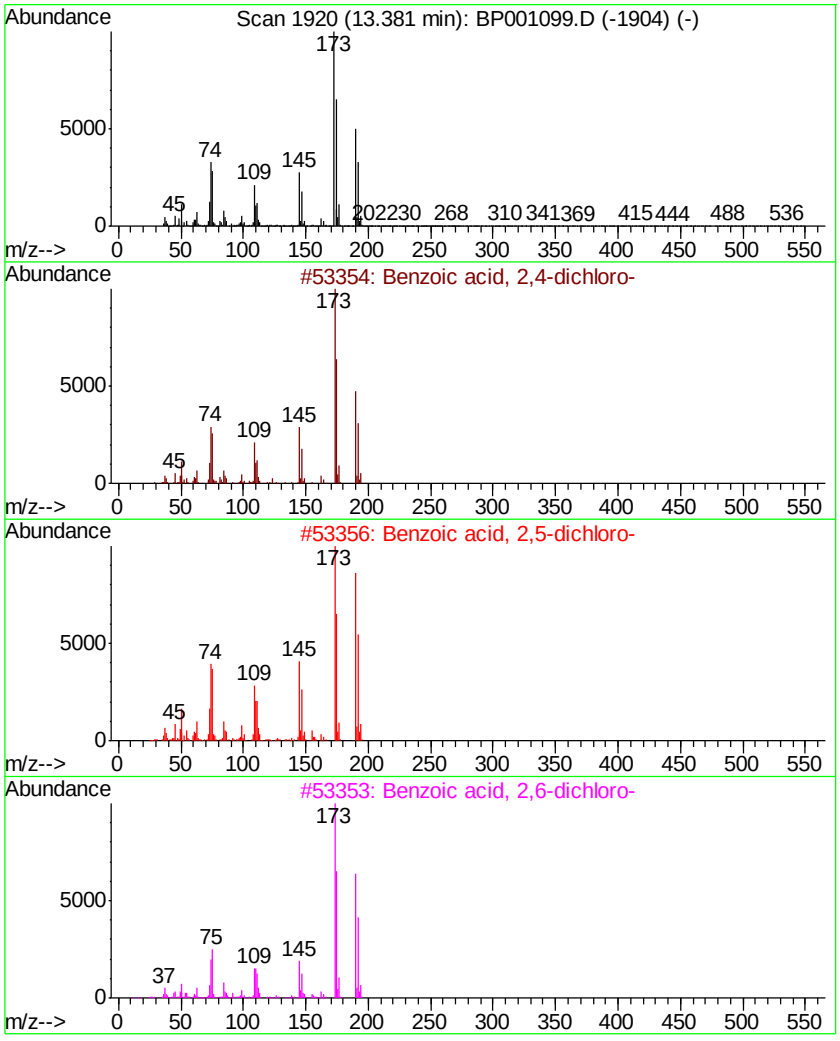
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

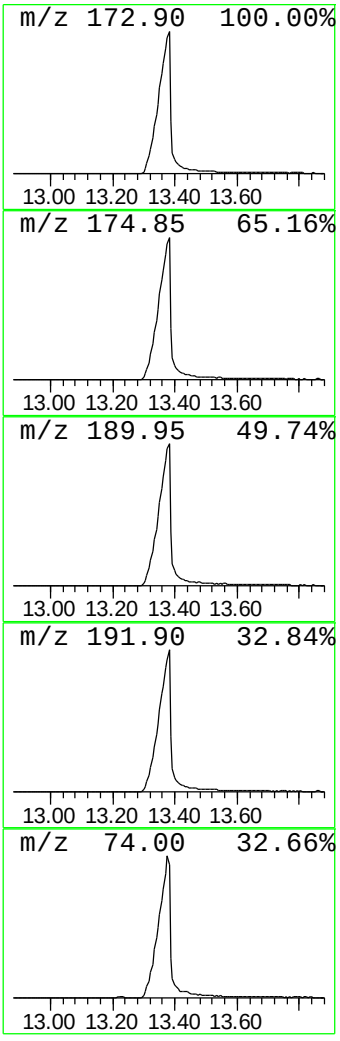
****

Peak Number 4 Benzoic acid, 2,4-dichloro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.38	60.17 ng	5818260	Acenaphthene-d10	13.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2,4-dichloro-	190	C7H4Cl2O2	000050-84-0	99
2	Benzoic acid, 2,5-dichloro-	190	C7H4Cl2O2	000050-79-3	97
3	Benzoic acid, 2,6-dichloro-	190	C7H4Cl2O2	000050-30-6	96
4	Benzoic acid, 3,4-dichloro-	190	C7H4Cl2O2	000051-44-5	86
5	Ethanone, 1-(2,4-dichlorophenyl)-	188	C8H6Cl2O	002234-16-4	72





Library Search Compound Report

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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : CALVTANK-1-20191121

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP112719.M
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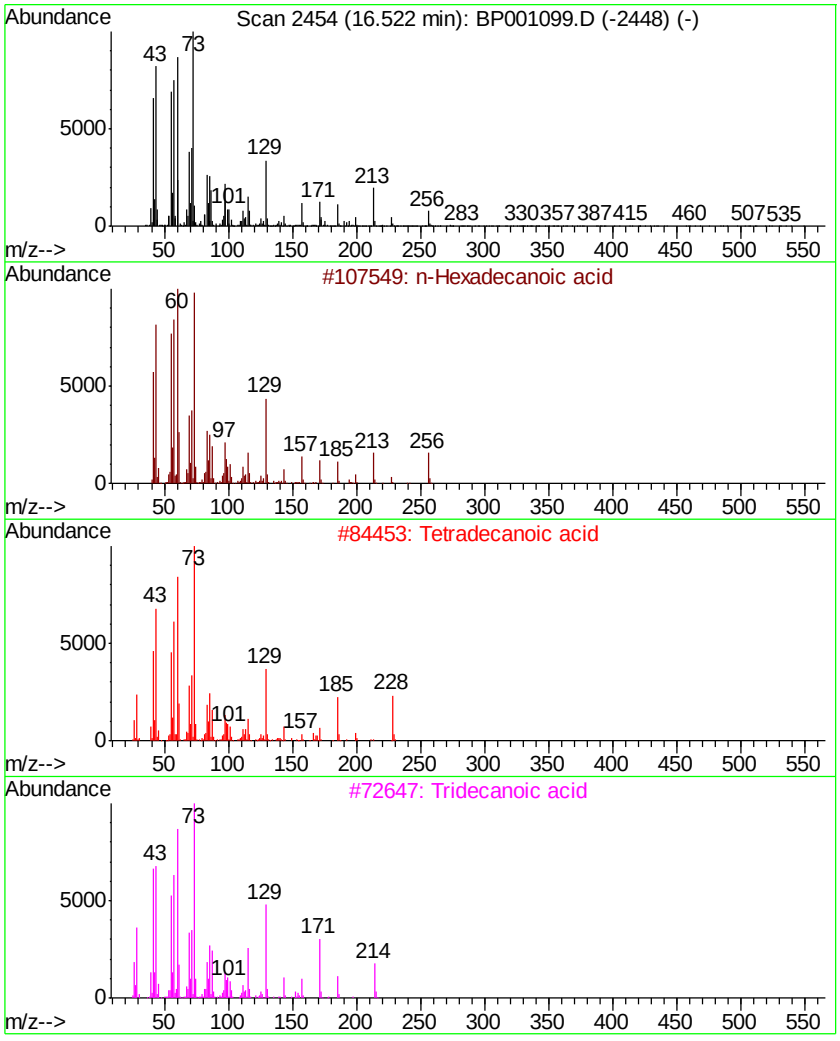
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

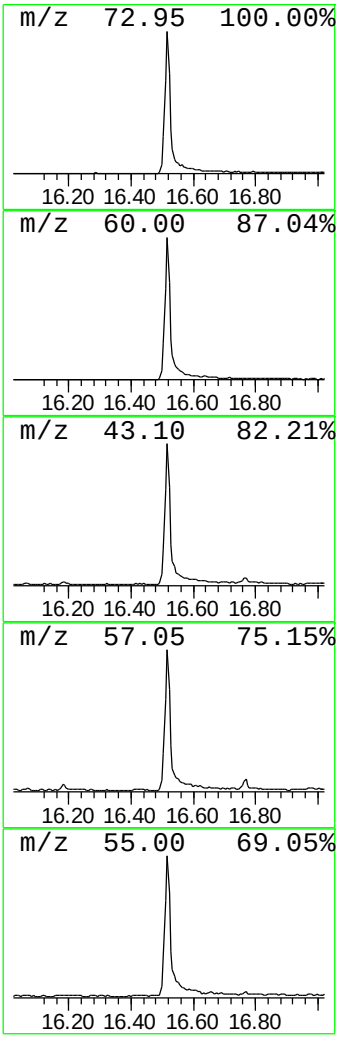
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.52	11.35 ng	1129490	Phenanthrene-d10	15.62

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	95
3	Tridecanoic acid	214	C13H26O2	000638-53-9	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5	Undecanoic acid	186	C11H22O2	000112-37-8	64





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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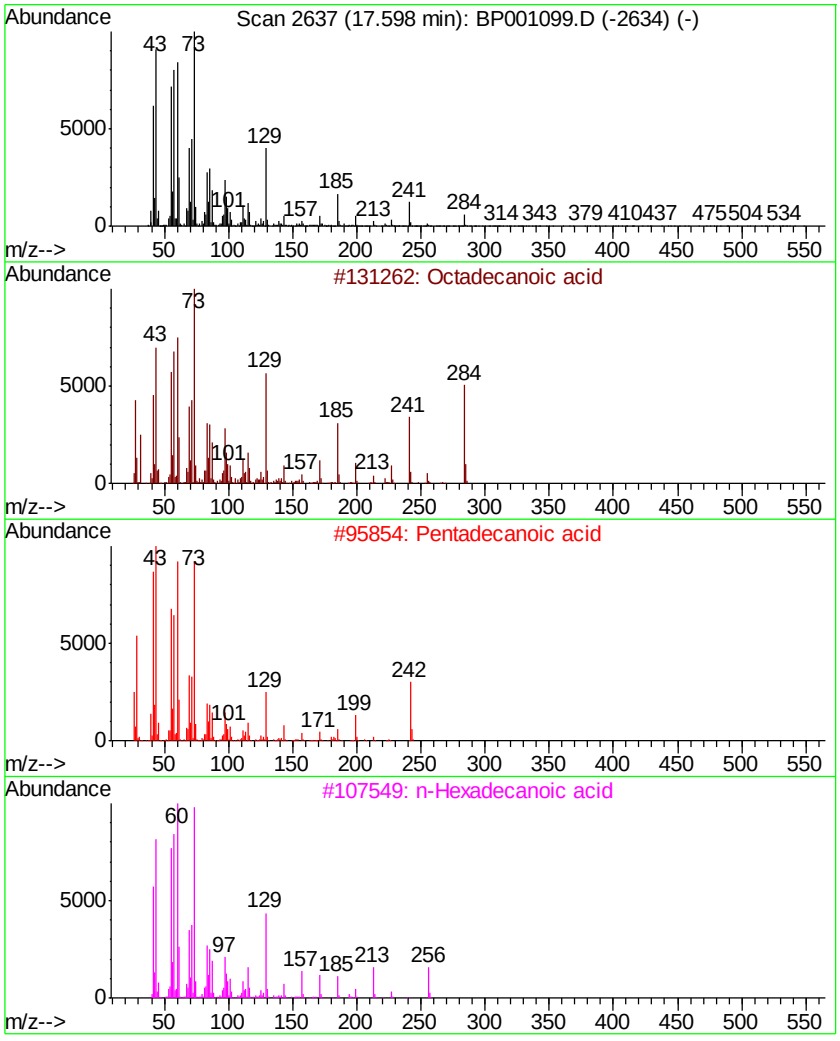
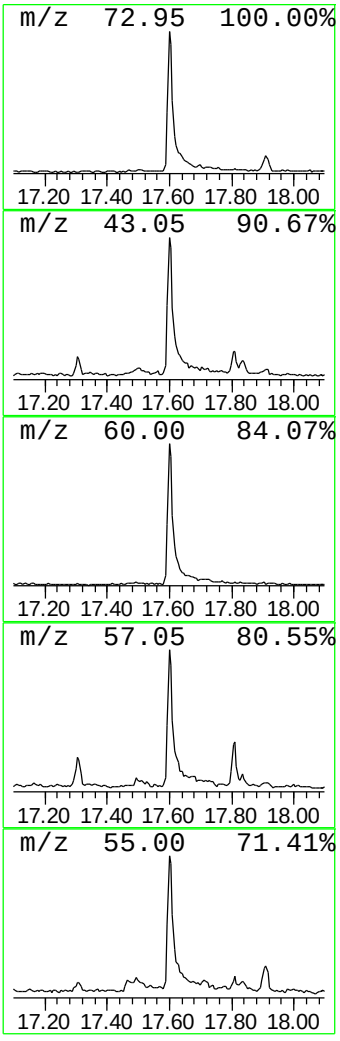
****

Peak Number 6 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.60	5.31 ng	448767	Chrysene-d12	19.26

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	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64





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Instrument : BNA_P
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

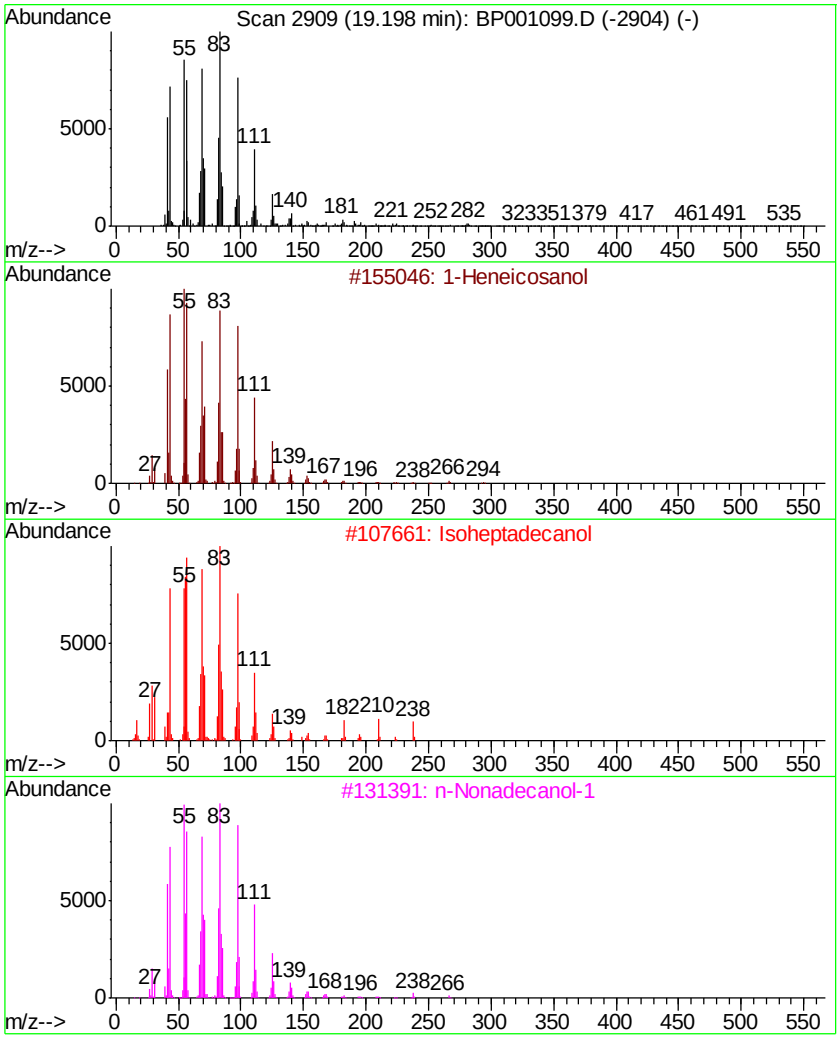
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

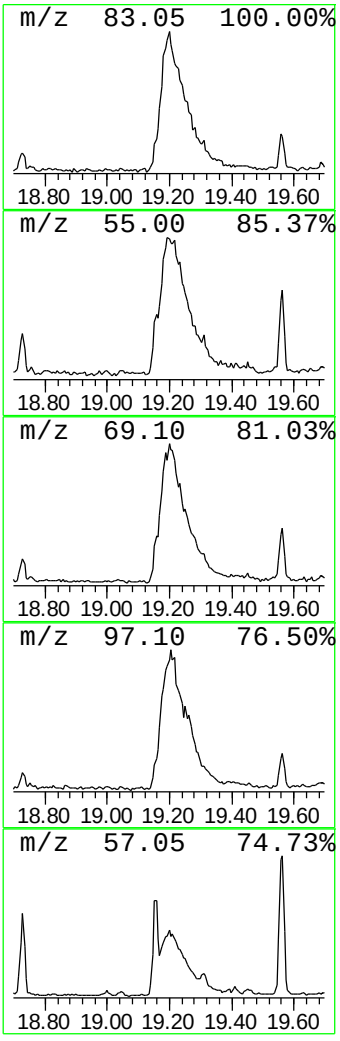
****

Peak Number 7 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.20	5.79 ng	489345	Chrysene-d12	19.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	Isoheptadecanol	256	C17H36O	057289-07-3	91
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
4	n-Heptadecanol-1	256	C17H36O	001454-85-9	87
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	83





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Instrument : BNA_P
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP112719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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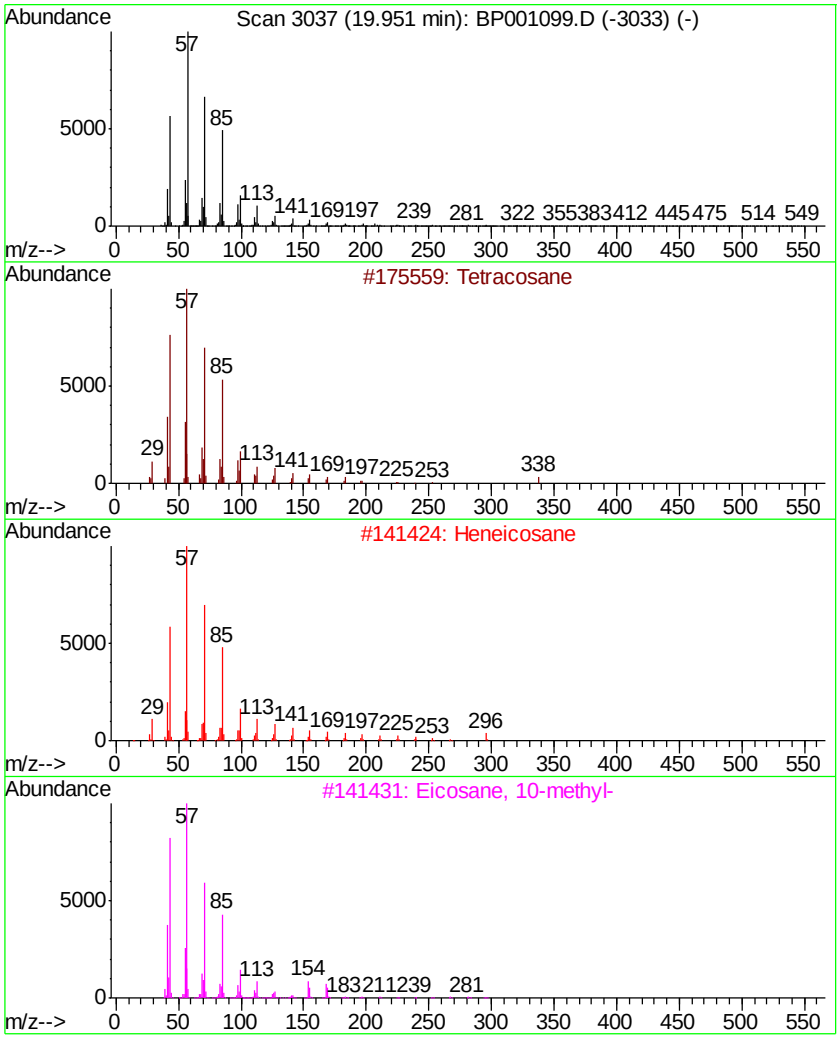
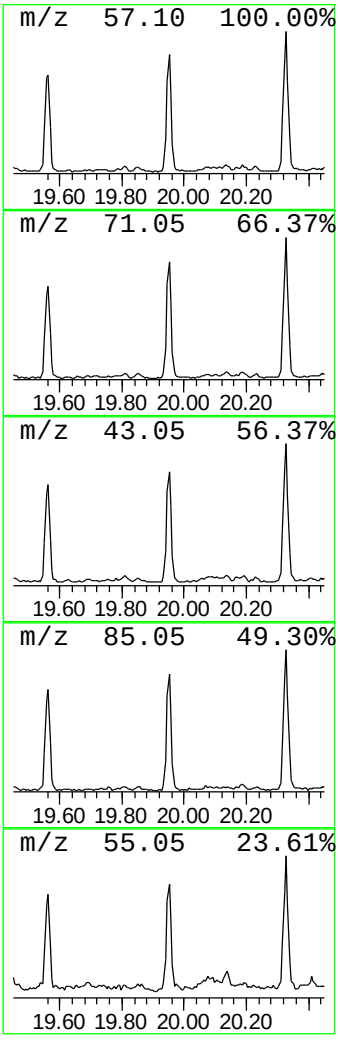
Peak Number 8 Eicosane, 10-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.95	2.39 ng	201732	Chrysene-d12	19.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	95
2	Heneicosane	296	C21H44	000629-94-7	94
3	Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
4	Pentacosane	352	C25H52	000629-99-2	93
5	Hexacosane	366	C26H54	000630-01-3	91





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Acq On : 28 Nov 2019 00:36
Operator : JU
Sample : K6008-01
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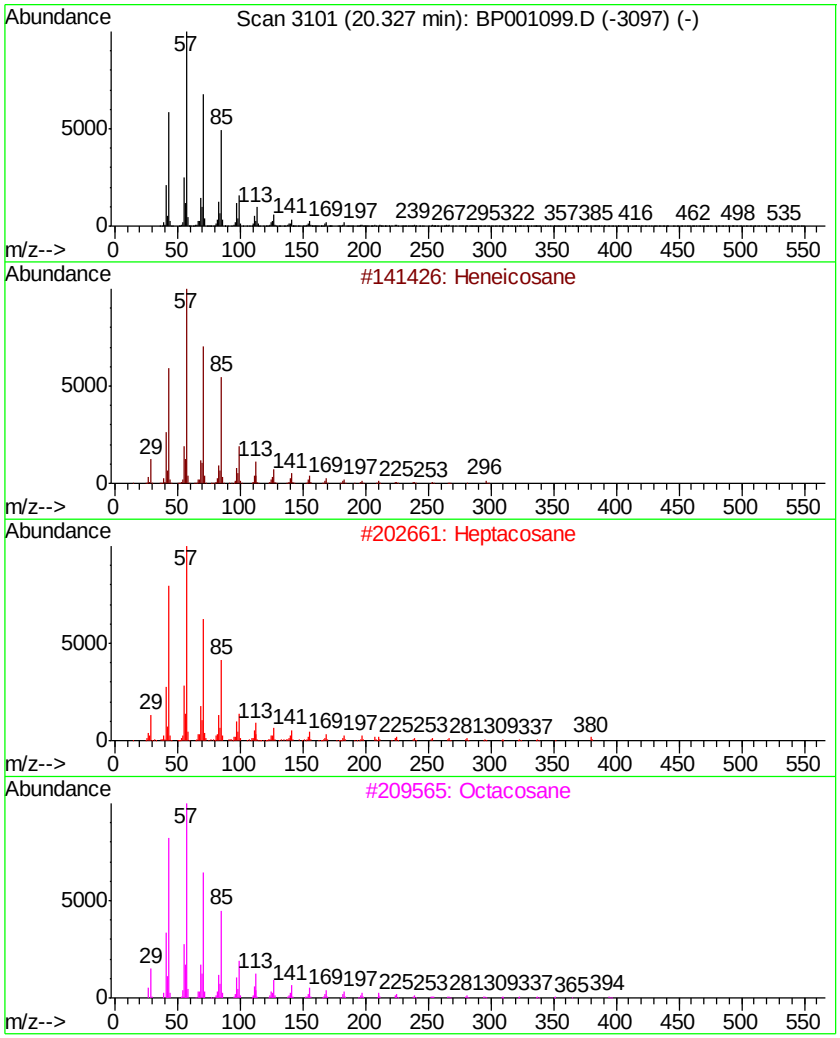
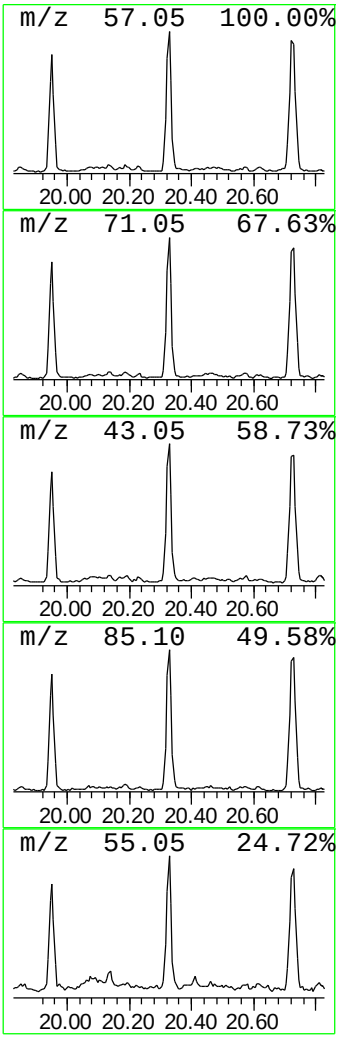
Peak Number 9 Heptacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.33	3.24 ng	248642	Perylene-d12	21.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Heptacosane	380	C27H56	000593-49-7	91
3	Octacosane	394	C28H58	000630-02-4	87
4	Nonadecane	268	C19H40	000629-92-5	86
5	Docosane	310	C22H46	000629-97-0	83





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Data File : BP001099.D
Acq On : 28 Nov 2019 00:36
Operator : JU
Sample : K6008-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : CALVTANK-1-20191121

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP112719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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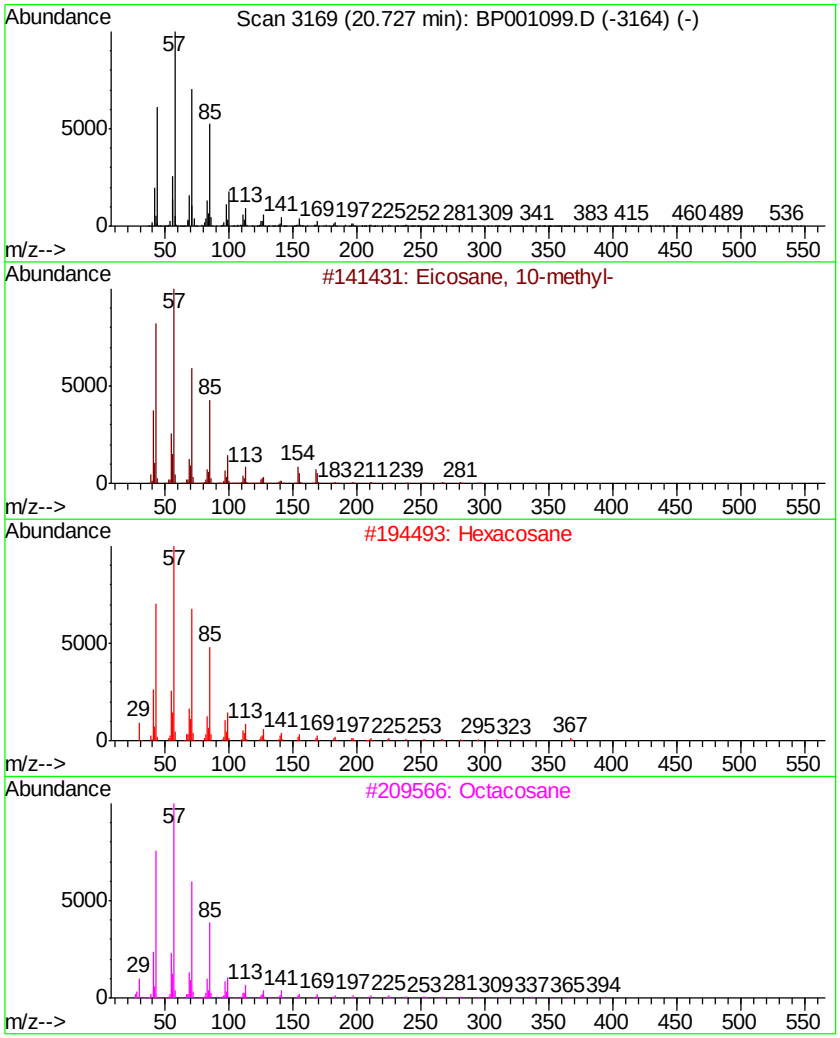
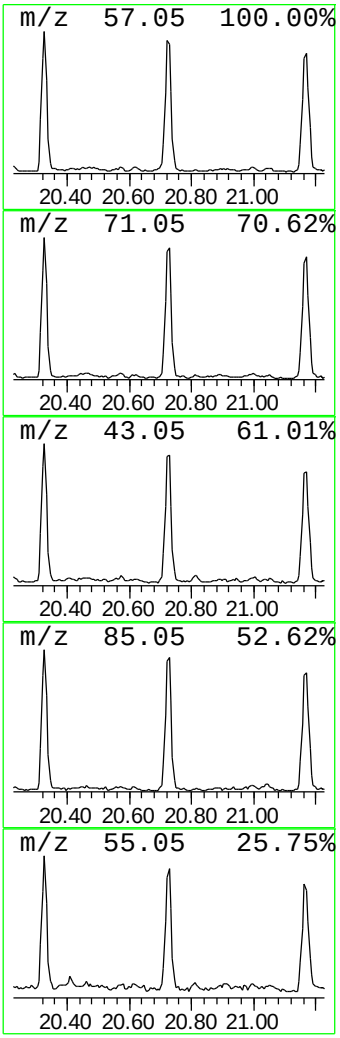
Peak Number 10 Heptadecane, 9-octyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.73	3.83 ng	293582	Perylene-d12	21.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
2	Hexacosane	366	C26H54	000630-01-3	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Heptadecane	240	C17H36	000629-78-7	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





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Data File : BP001099.D
Acq On : 28 Nov 2019 00:36
Operator : JU
Sample : K6008-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : CALVTANK-1-20191121

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP112719.M
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TIC Integration Parameters: LSCINT.P

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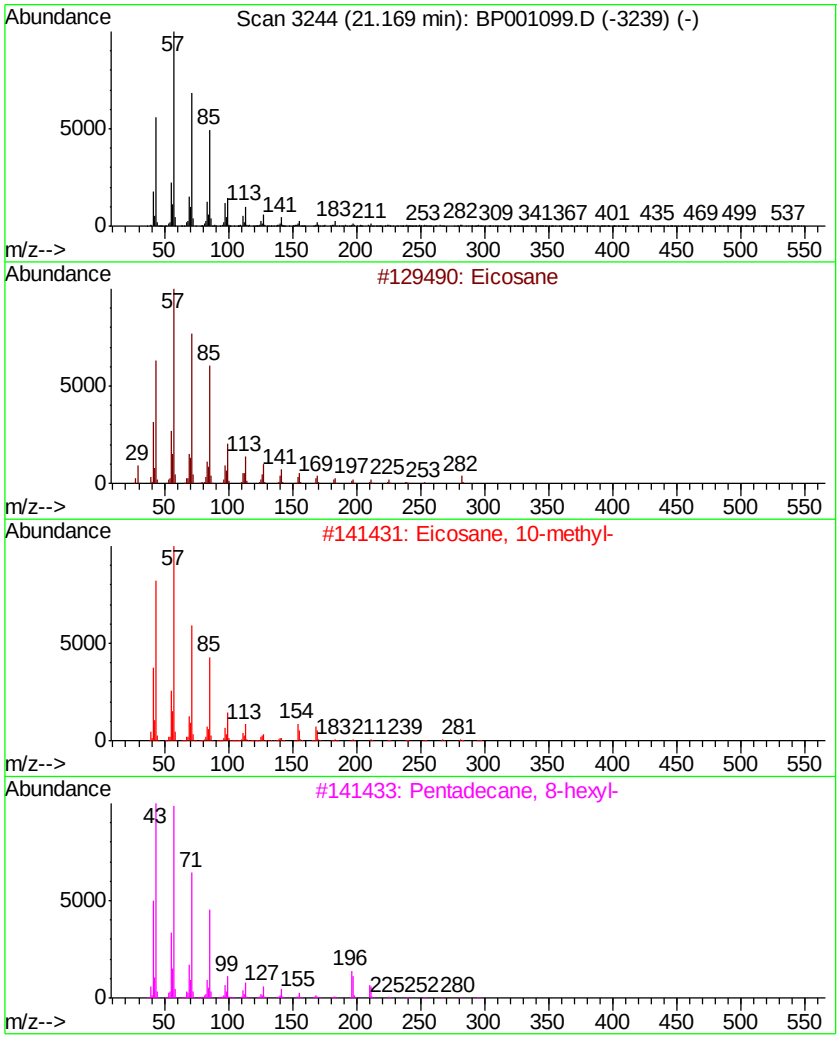
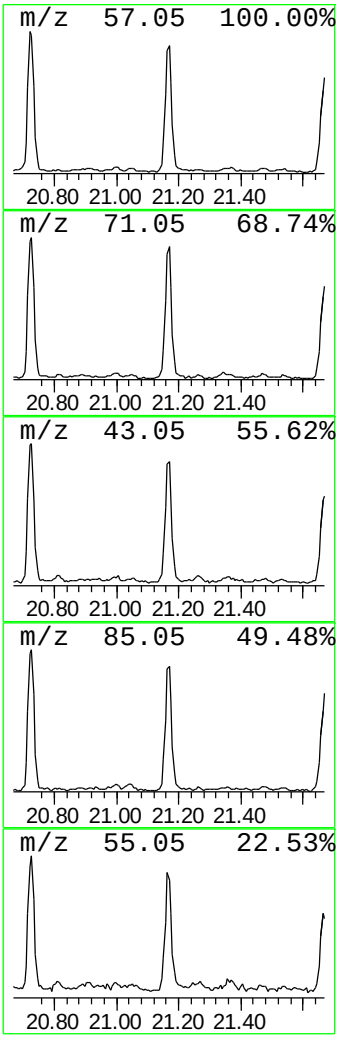
Peak Number 11 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.17	3.47 ng	266023	Perylene-d12	21.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Eicosane, 10-methyl-	296	C21H44	054833-23-7	94
3	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	94
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Hexacosane	366	C26H54	000630-01-3	91





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Data File : BP001099.D
Acq On : 28 Nov 2019 00:36
Operator : JU
Sample : K6008-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : CALVTANK-1-20191121

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP112719.M
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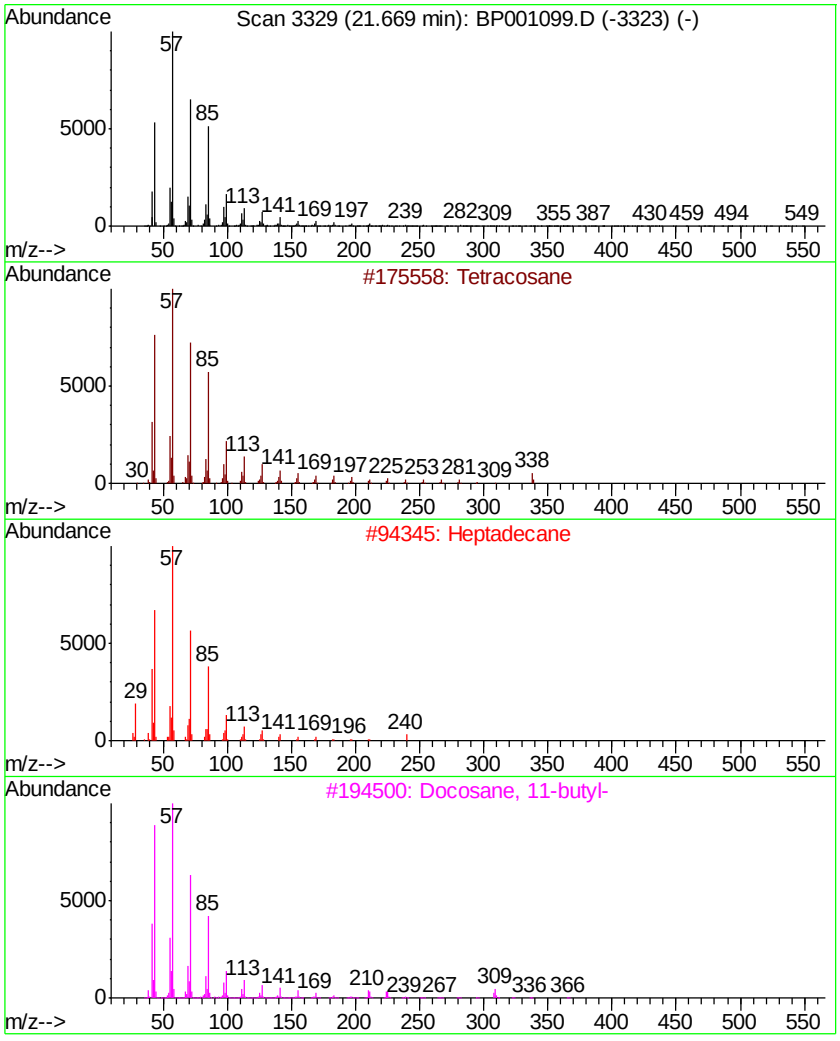
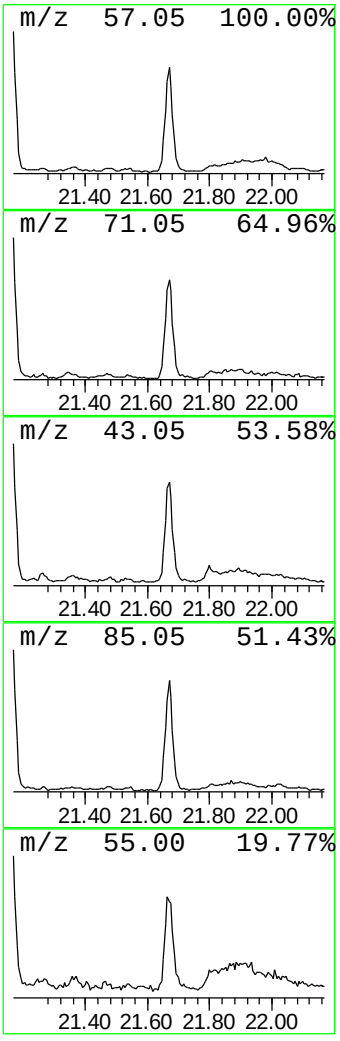
Peak Number 12 Tetracosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.67	3.17 ng	242875	Perylene-d12	21.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	94
2	Heptadecane	240	C17H36	000629-78-7	93
3	Docosane, 11-butyl-	366	C26H54	013475-76-8	93
4	Heneicosane	296	C21H44	000629-94-7	91
5	Octacosane	394	C28H58	000630-02-4	91





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Data File : BP001099.D
Acq On : 28 Nov 2019 00:36
Operator : JU
Sample : K6008-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : CALVTANK-1-20191121

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP112719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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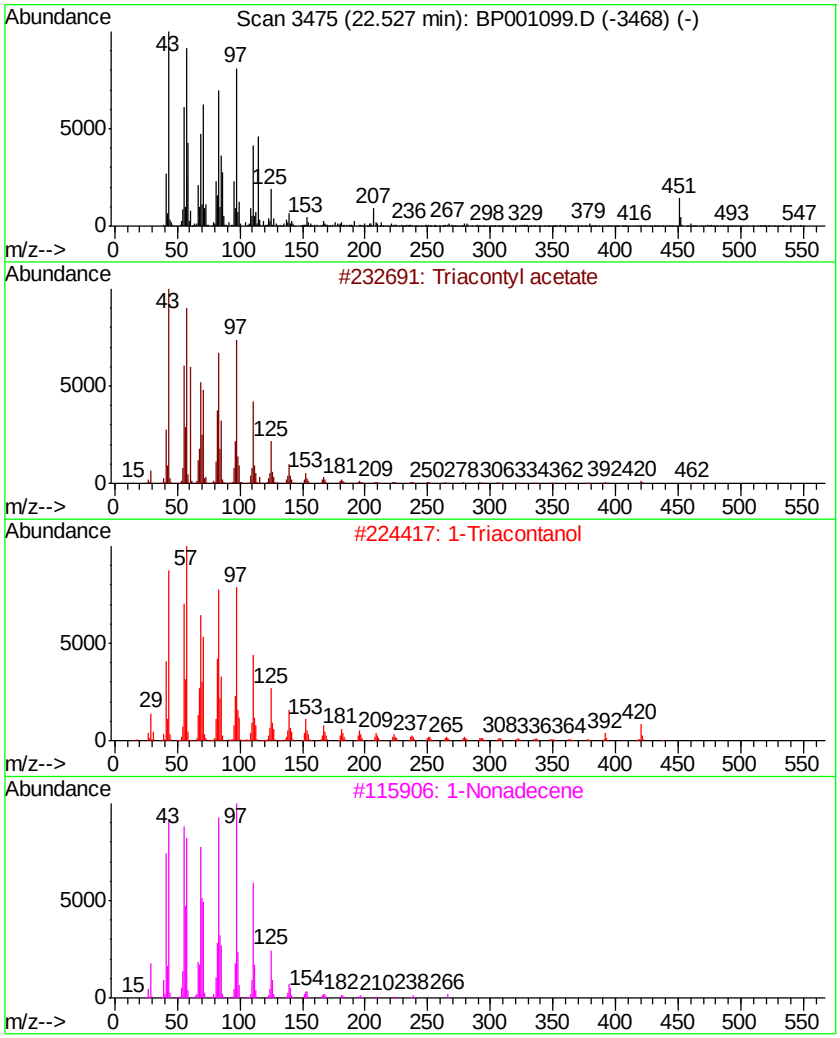
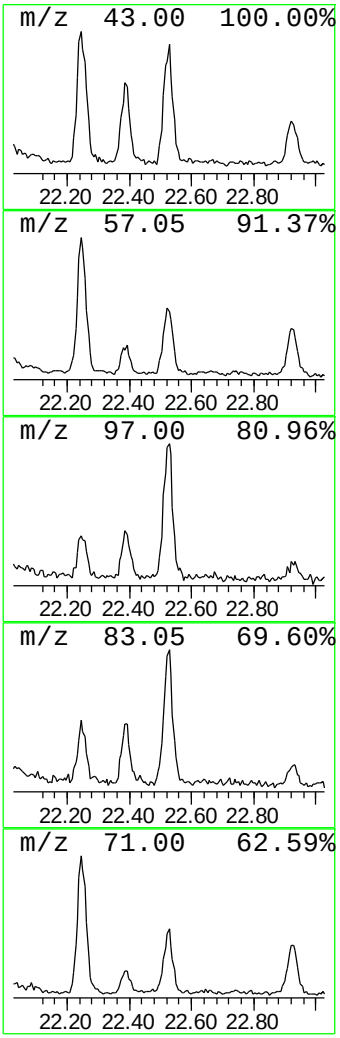
Peak Number 13 Triacontyl acetate Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.53	2.31 ng	177119	Perylene-d12	21.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontyl acetate	480	C32H64O2	041755-58-2	55
2	1-Triacontanol	438	C30H62O	000593-50-0	46
3	1-Nonadecene	266	C19H38	018435-45-5	38
4	Eicosane, 9-cyclohexyl-	364	C26H52	004443-61-2	25
5	Cyclohexane, (1-hexyltetradecyl)-	364	C26H52	004443-60-1	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_P\DATA\BP112719\
Data File : BP001099.D
Acq On : 28 Nov 2019 00:36
Operator : JU
Sample : K6008-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : CALVTANK-1-20191121

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP112719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.64	11.3	ng	655196	1	8.33	1163610	20.0
unknown7.96	7.96	91.5	ng	5326240	1	8.33	1163610	20.0
Benzoic acid, 2,4...	13.38	60.2	ng	5818260	3	13.23	1933890	20.0
n-Hexadecanoic acid	16.52	11.4	ng	1129490	4	15.62	1989630	20.0
Octadecanoic acid	17.60	5.3	ng	448767	5	19.26	1689740	20.0
1-Heneicosanol	19.20	5.8	ng	489345	5	19.26	1689740	20.0
Eicosane, 10-methyl-	19.95	2.4	ng	201732	5	19.26	1689740	20.0
Heptacosane	20.33	3.2	ng	248642	6	21.05	1532680	20.0
Heptadecane, 9-oc...	20.73	3.8	ng	293582	6	21.05	1532680	20.0
Eicosane	21.17	3.5	ng	266023	6	21.05	1532680	20.0
Tetracosane	21.67	3.2	ng	242875	6	21.05	1532680	20.0
Triacontyl acetate	22.53	2.3	ng	177119	6	21.05	1532680	20.0