

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP093020\
 Data File : BP003416.D
 Acq On : 30 Sep 2020 16:39
 Operator : CG/JU
 Sample : PB131959BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 PB131959BL

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-BP091520.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP003416.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.152	379	385	405	rBV	638839	1062634	27.75%	6.583%
2	6.740	648	655	682	rBV	607714	1120670	29.26%	6.943%
3	7.540	784	791	802	rBV	137882	230149	6.01%	1.426%
4	8.687	979	986	1006	rBV	397343	763058	19.93%	4.727%
5	10.316	1256	1263	1281	rBV	162417	328838	8.59%	2.037%
6	12.804	1679	1686	1700	rBV	1263429	2033272	53.09%	12.597%
7	13.669	1827	1833	1845	rBV	31874	61990	1.62%	0.384%
8	14.193	1916	1922	1943	rBV	313398	506852	13.24%	3.140%
9	15.698	2171	2178	2201	rBV	864877	1527208	39.88%	9.462%
10	16.951	2385	2391	2404	rBV	395491	638305	16.67%	3.955%
11	18.151	2590	2595	2599	rBV2	25926	46439	1.21%	0.288%
12	18.622	2666	2675	2685	rBV8	14156	55914	1.46%	0.346%
13	19.533	2824	2830	2840	rBV	3070810	3829586	100.00%	23.725%
14	19.704	2852	2859	2865	rBV3	31559	85201	2.22%	0.528%
15	20.533	2995	3000	3010	rBV2	56422	152933	3.99%	0.947%
16	20.786	3039	3043	3049	rBV2	194018	292153	7.63%	1.810%
17	20.839	3049	3052	3061	rVB	126288	182463	4.76%	1.130%
18	21.057	3084	3089	3101	rBV	631466	875416	22.86%	5.423%
19	21.222	3113	3117	3118	rBV2	35495	44700	1.17%	0.277%
20	21.245	3118	3121	3130	rVB3	61599	116181	3.03%	0.720%
21	21.639	3185	3188	3192	rBV	86418	103205	2.69%	0.639%
22	22.092	3261	3265	3272	rVB	168554	231831	6.05%	1.436%
23	22.592	3346	3350	3356	rBV	216603	317748	8.30%	1.969%
24	23.151	3440	3445	3453	rVB	219449	385528	10.07%	2.388%
25	23.251	3456	3462	3474	rVB2	389249	815346	21.29%	5.051%
26	23.792	3549	3554	3563	rVB	171649	333606	8.71%	2.067%

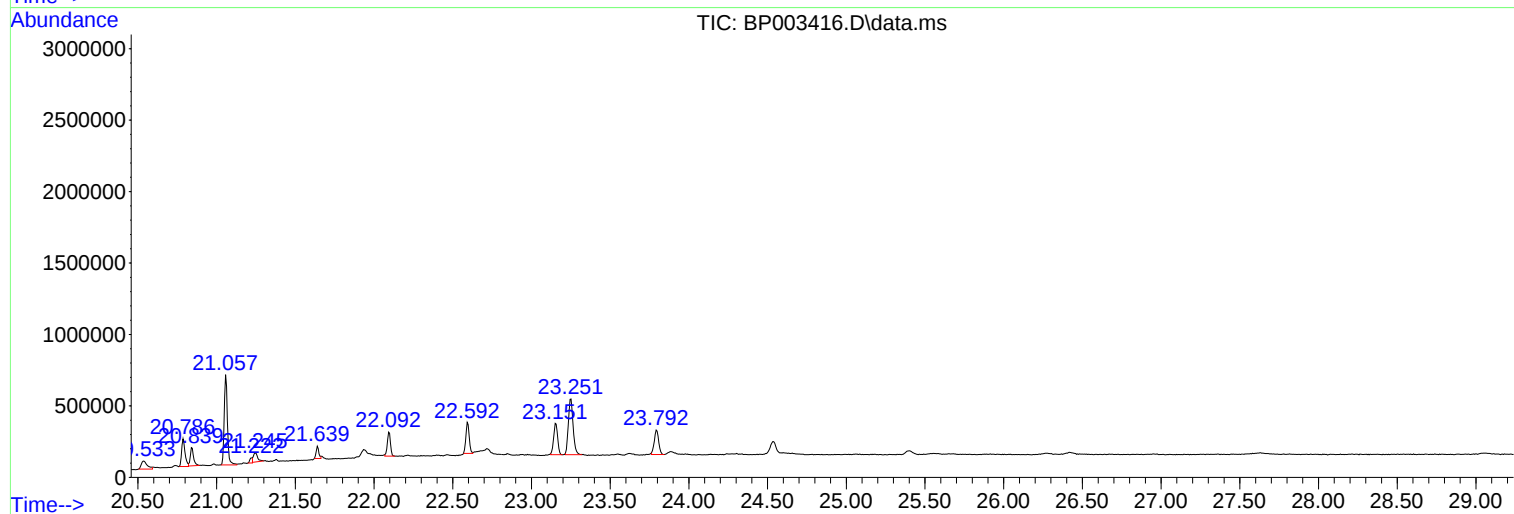
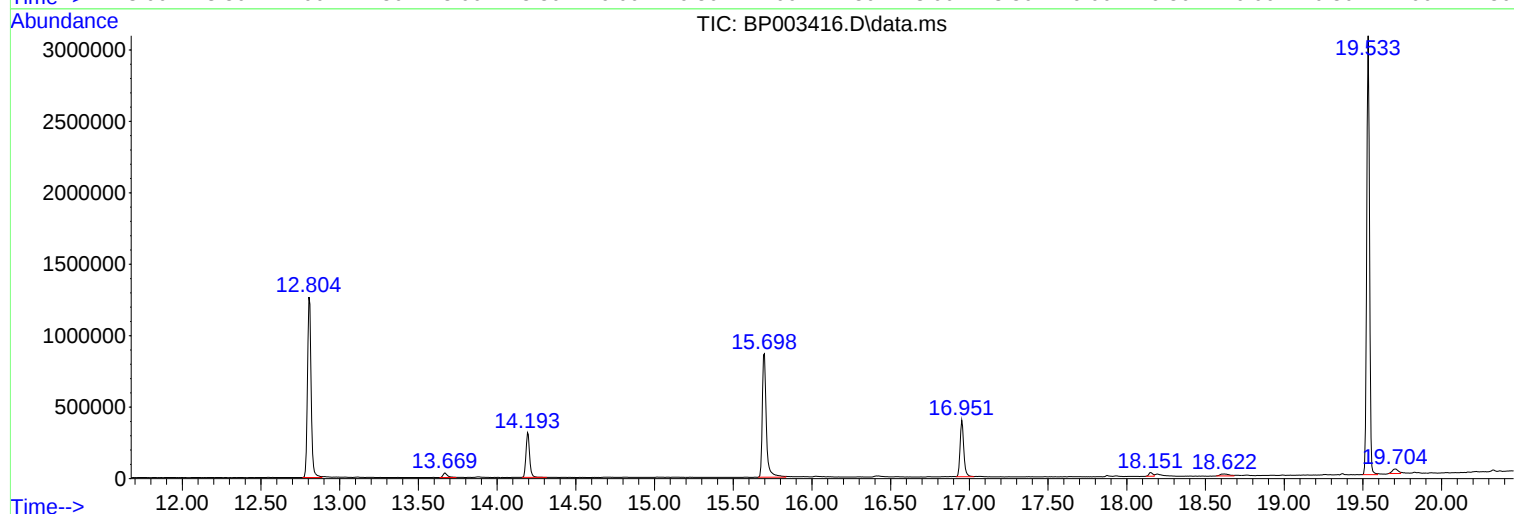
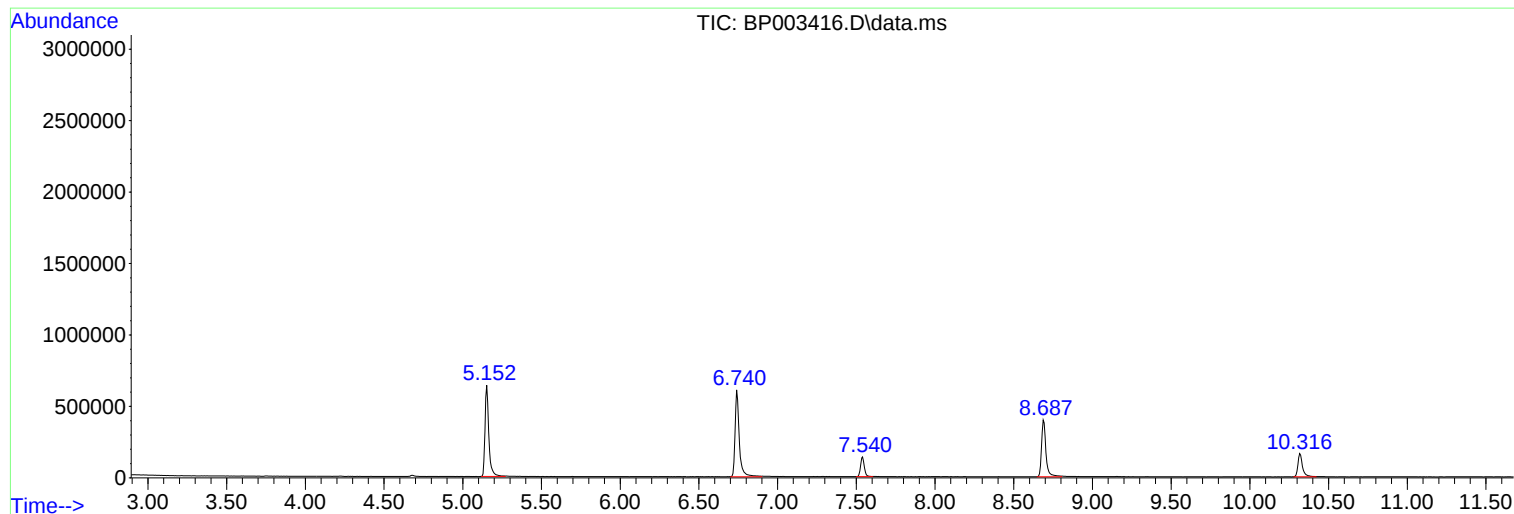
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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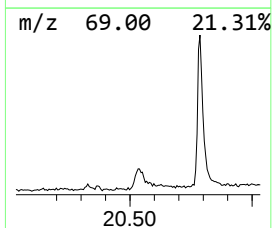
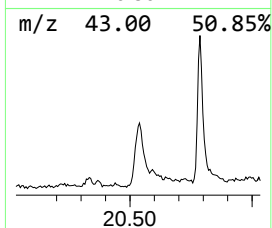
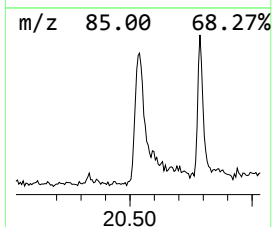
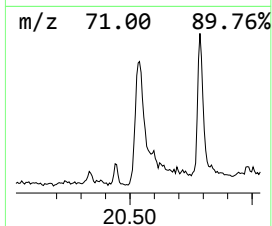
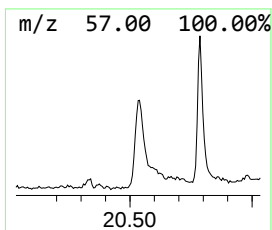
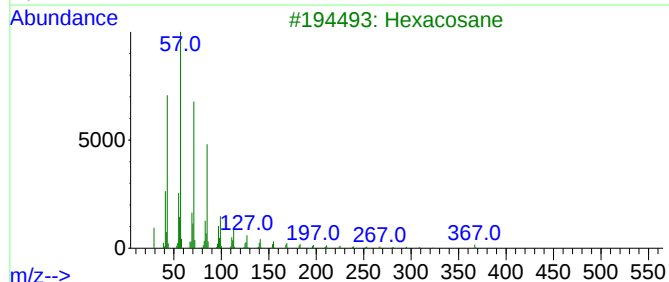
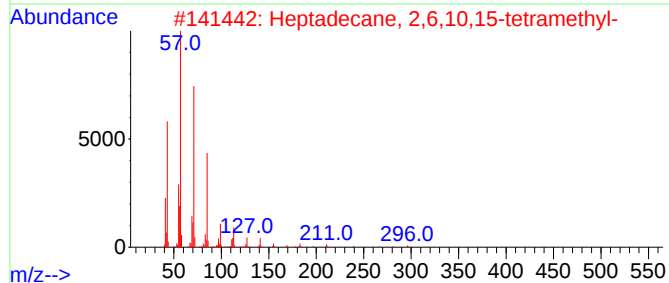
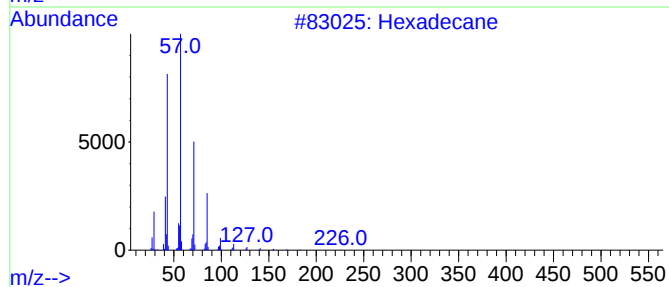
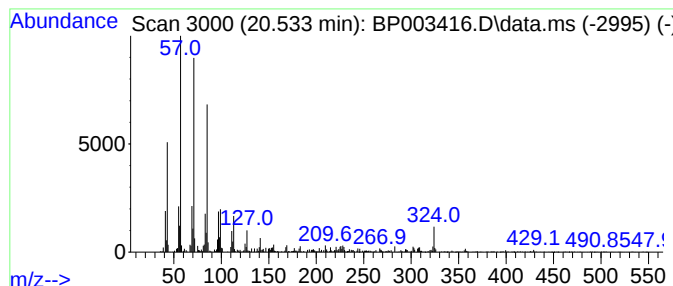
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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Peak Number 1 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.533	3.49 ng	152933	Chrysene-d12	21.057

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecane	226	C16H34	000544-76-3	93
2		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90
3		Hexacosane	366	C26H54	000630-01-3	87
4		2-methyloctacosane	408	C29H60	1000376-72-8	86
5		Heptacosane	380	C27H56	000593-49-7	86



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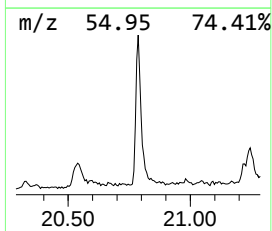
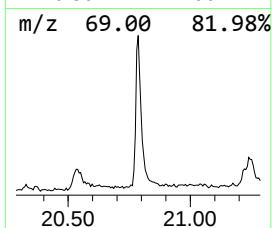
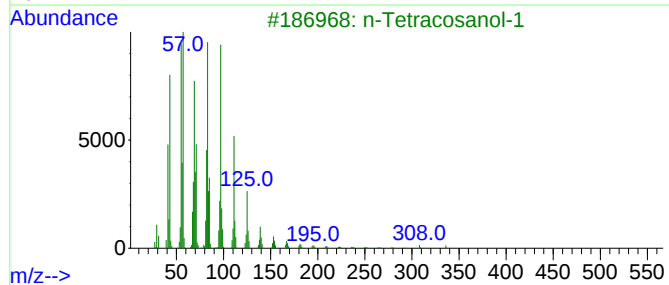
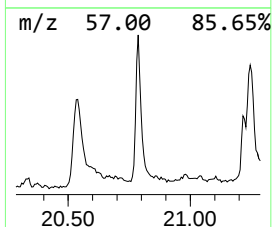
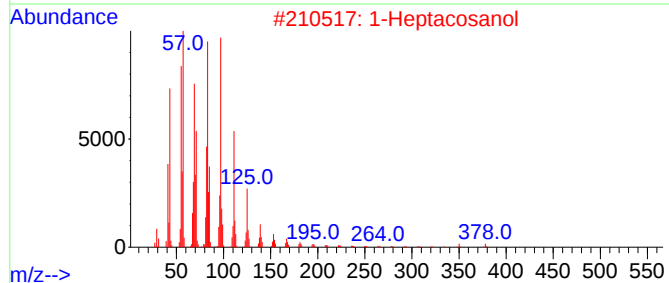
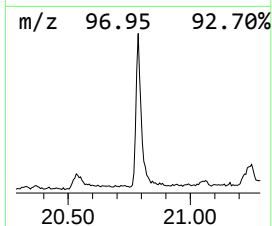
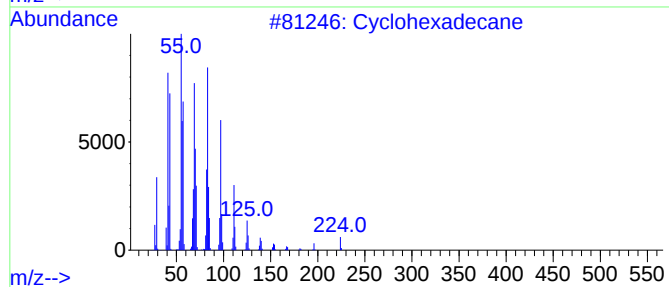
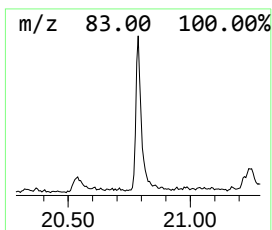
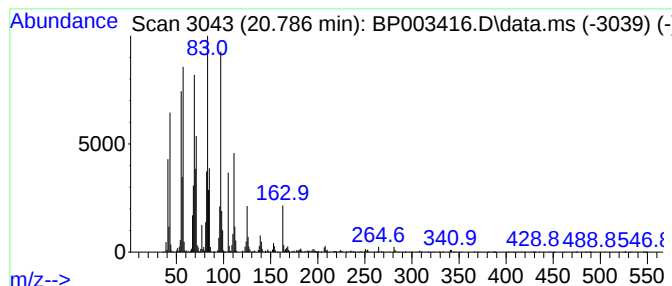
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Cyclohexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.786	6.67 ng	292153	Chrysene-d12	21.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	93
2			1-Heptacosanol	396	C27H56O	002004-39-9	93
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	93
4			E-14-Hexadecenal	238	C16H30O	330207-53-9	91
5			1-Triacontanol	438	C30H62O	000593-50-0	91



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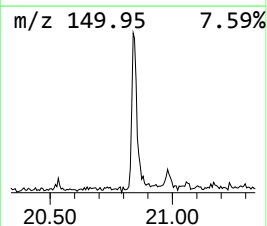
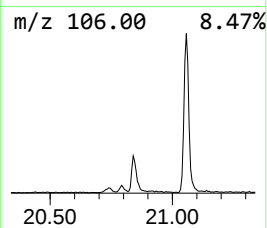
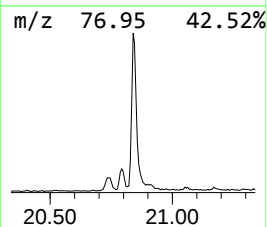
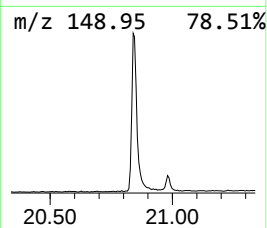
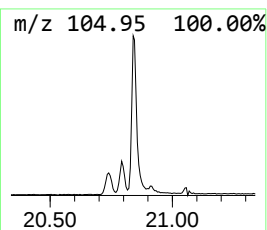
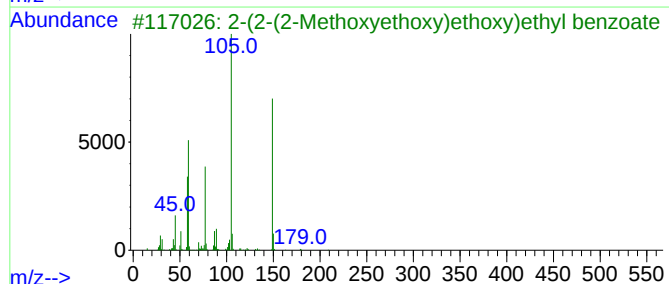
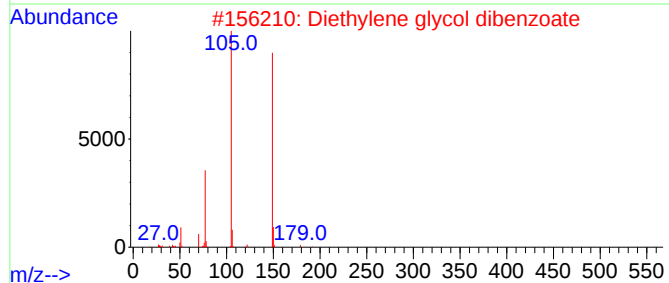
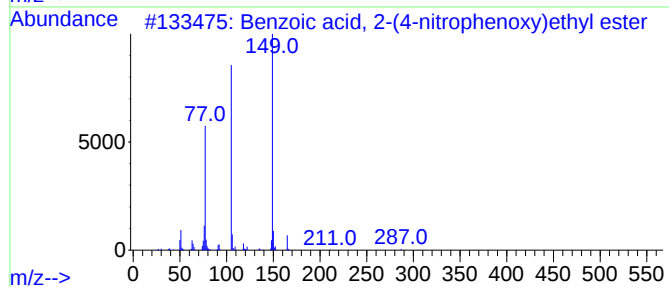
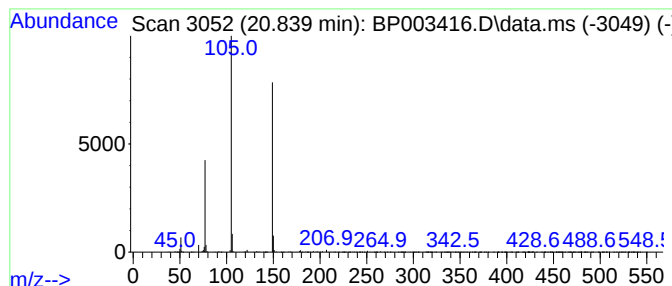
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Benzoic acid, 2-(4-nitrophe... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.839	4.17 ng	182463	Chrysene-d12	21.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	78
2			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	72
3			2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	64
4			2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	64
5			3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	64



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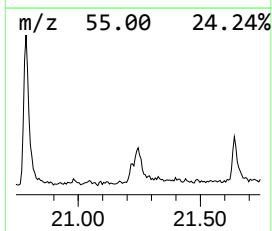
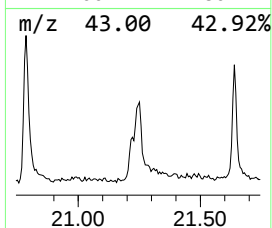
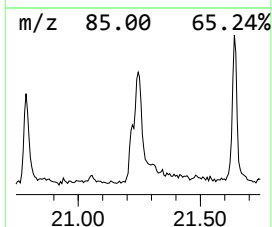
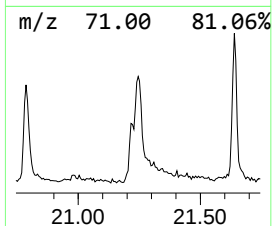
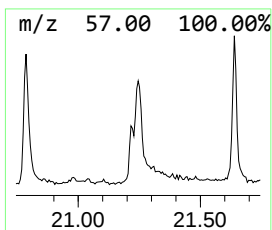
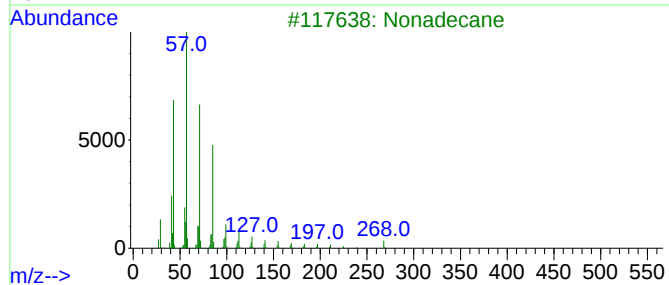
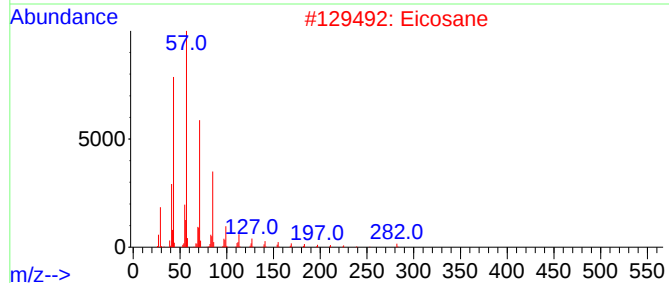
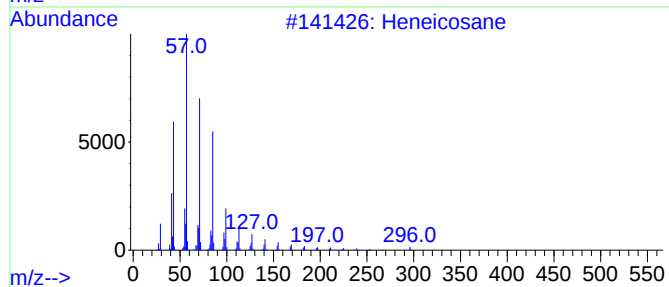
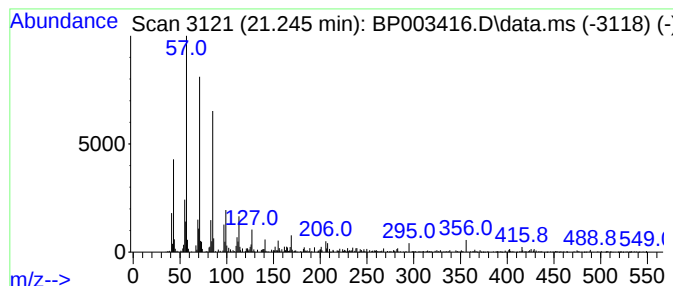
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.245	2.65 ng	116181	Chrysene-d12	21.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	87
2			Eicosane	282	C20H42	000112-95-8	87
3			Nonadecane	268	C19H40	000629-92-5	87
4			Hexacosane	366	C26H54	000630-01-3	87
5			Hexadecane	226	C16H34	000544-76-3	83



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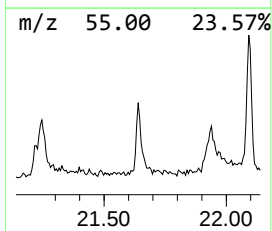
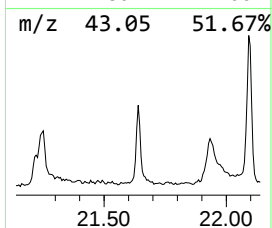
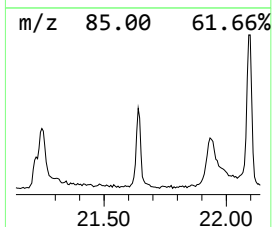
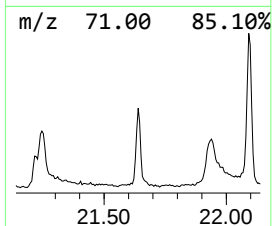
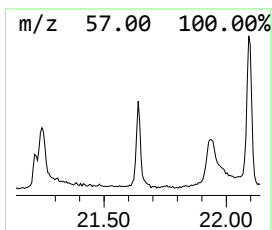
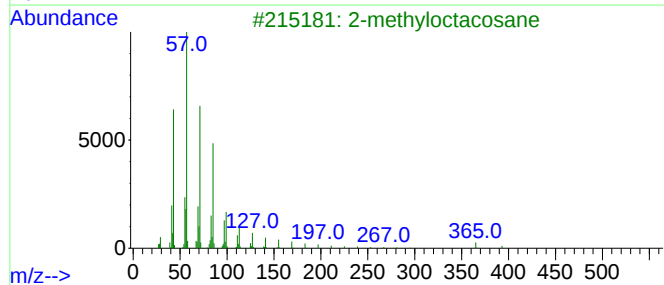
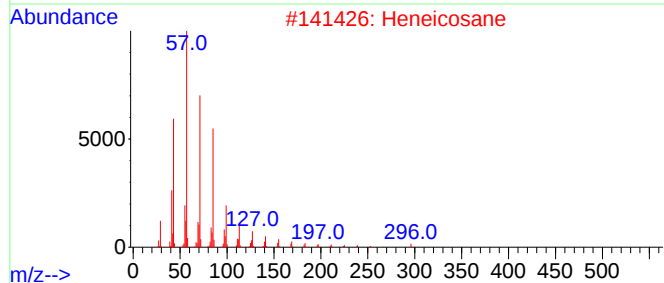
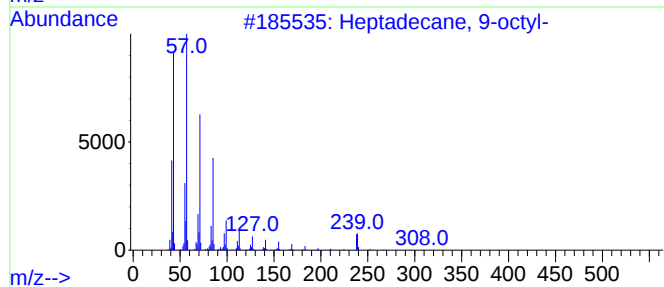
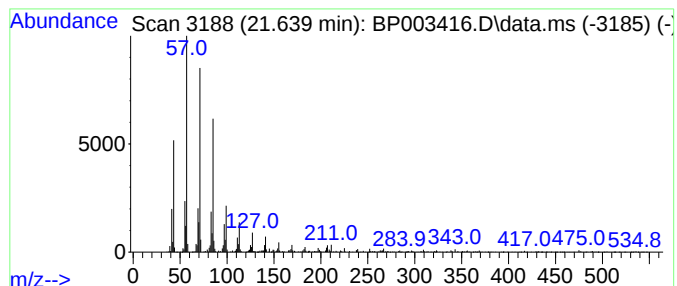
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Heptadecane, 9-octyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.639	2.36 ng	103205	Chrysene-d12	21.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	93
2			Heneicosane	296	C21H44	000629-94-7	91
3			2-methyloctacosane	408	C29H60	1000376-72-8	91
4			Heptadecane, 8,8-dipentyl-	380	C27H56	055282-28-5	91
5			Hexacosane	366	C26H54	000630-01-3	91



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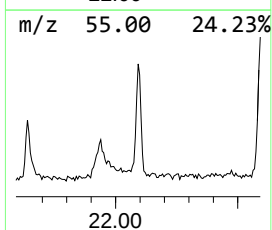
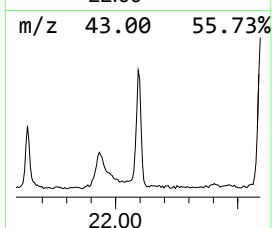
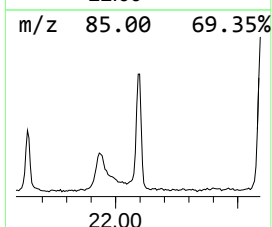
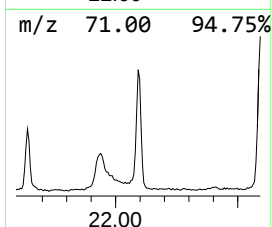
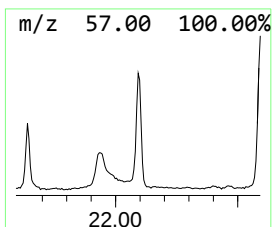
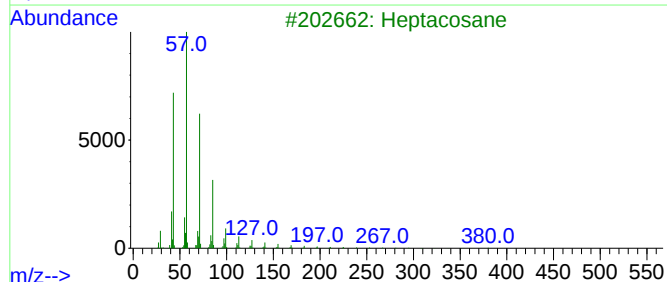
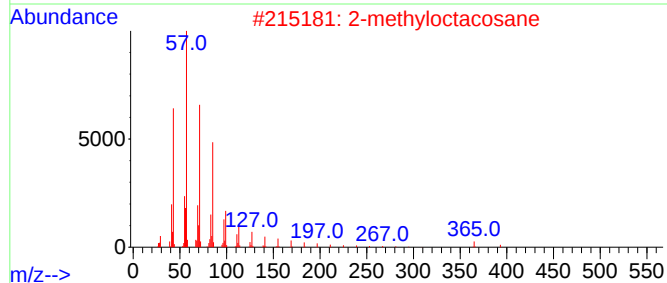
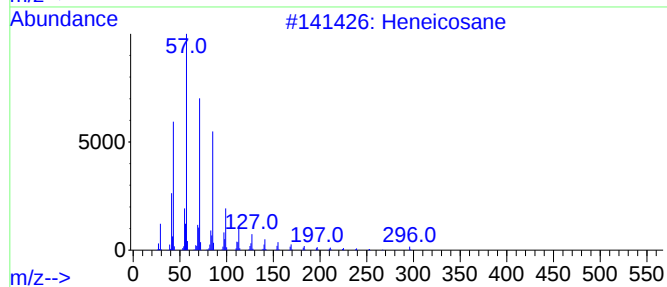
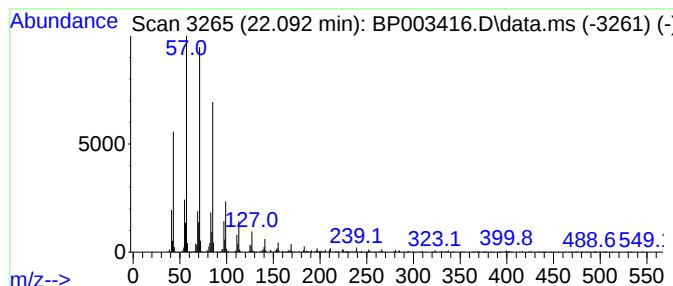
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.092	5.30 ng	231831	Chrysene-d12	21.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			2-methyloctacosane	408	C29H60	1000376-72-8	91
3			Heptacosane	380	C27H56	000593-49-7	91
4			Hexacosane	366	C26H54	000630-01-3	90
5			Heptadecane	240	C17H36	000629-78-7	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP093020\
Data File : BP003416.D
Acq On : 30 Sep 2020 16:39
Operator : CG/JU
Sample : PB131959BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PB131959BL

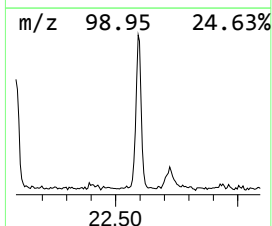
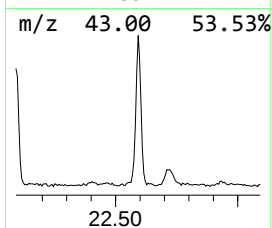
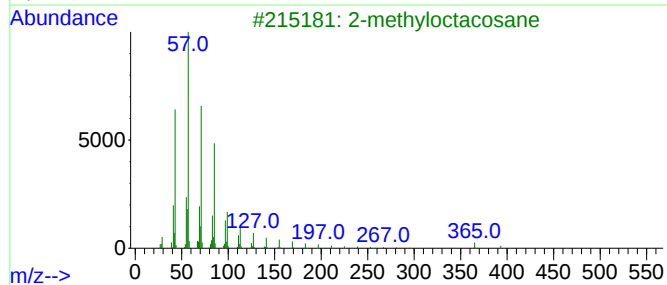
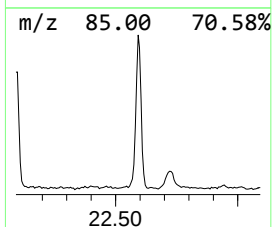
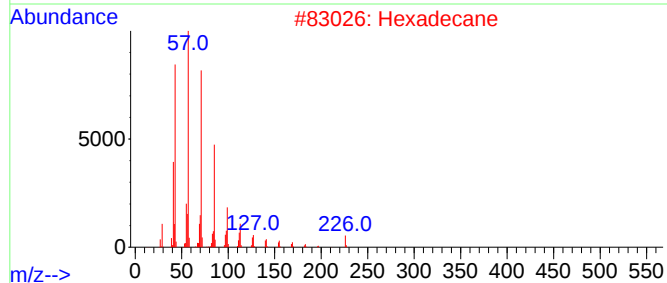
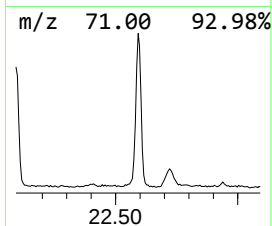
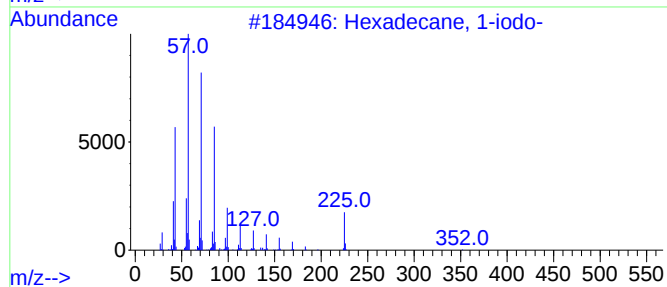
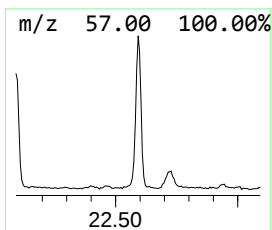
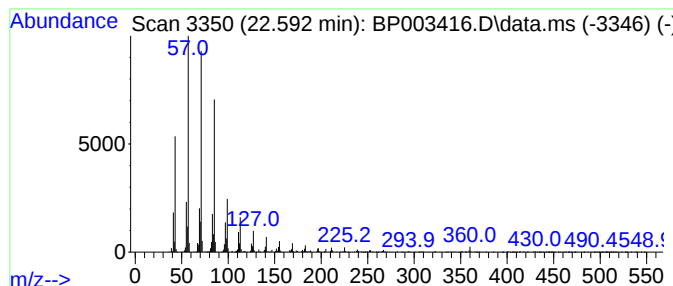
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecane, 1-iodo- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.592	7.79 ng	317748	Perylene-d12	23.251

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 1-iodo-			352	C16H33I	000544-77-4	93
2	Hexadecane			226	C16H34	000544-76-3	93
3	2-methyloctacosane			408	C29H60	1000376-72-8	91
4	Tetracosane			338	C24H50	000646-31-1	91
5	Triacontane			422	C30H62	000638-68-6	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP093020\
Data File : BP003416.D
Acq On : 30 Sep 2020 16:39
Operator : CG/JU
Sample : PB131959BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PB131959BL

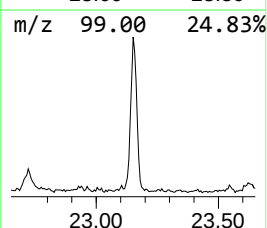
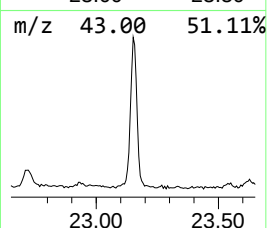
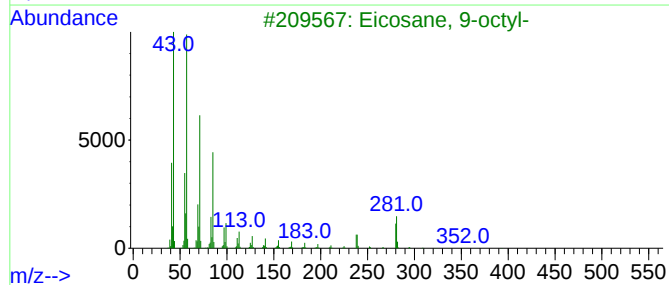
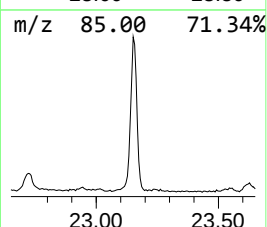
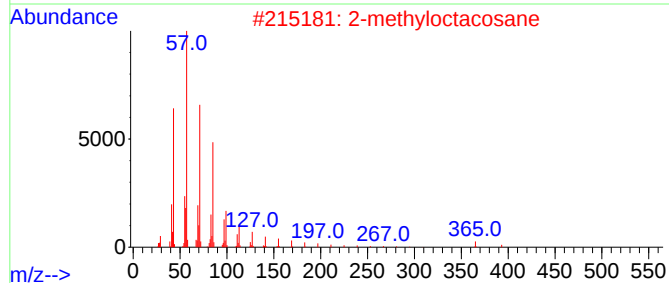
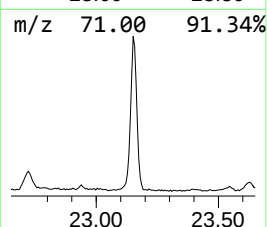
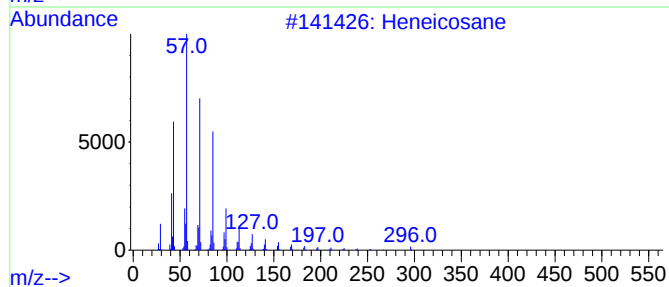
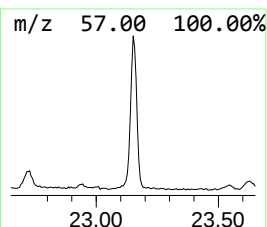
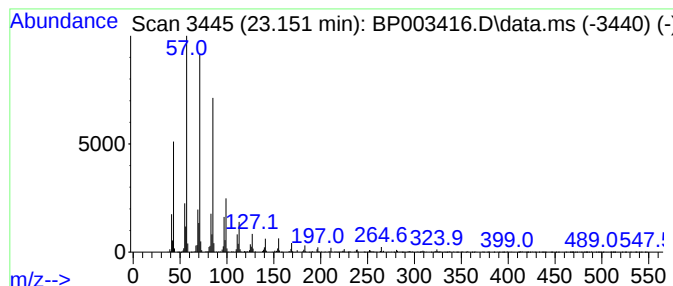
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.151	9.46 ng	385528	Perylene-d12	23.251

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			2-methyloctacosane	408	C29H60	1000376-72-8	91
3			Eicosane, 9-octyl-	394	C28H58	013475-77-9	90
4			Hexacosane	366	C26H54	000630-01-3	90
5			Tetracosane	338	C24H50	000646-31-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP093020\
Data File : BP003416.D
Acq On : 30 Sep 2020 16:39
Operator : CG/JU
Sample : PB131959BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PB131959BL

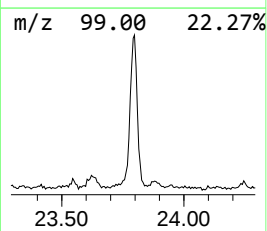
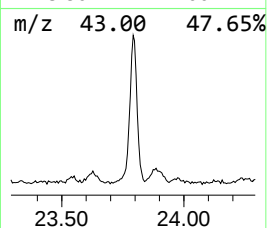
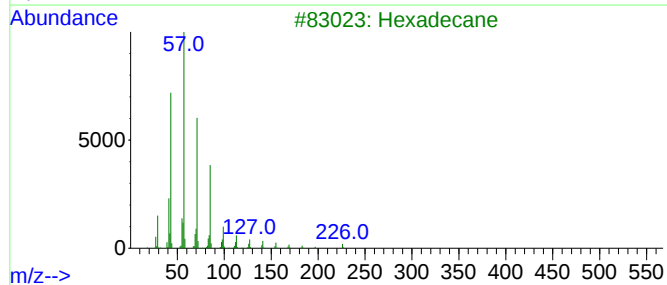
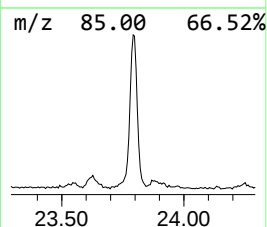
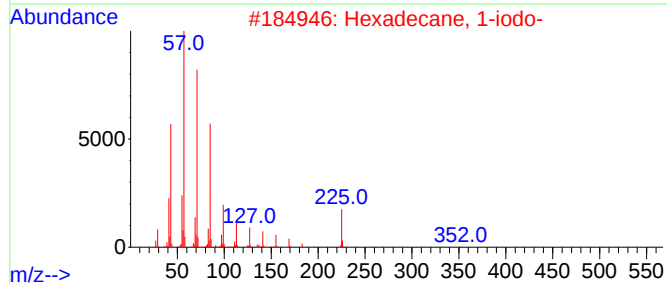
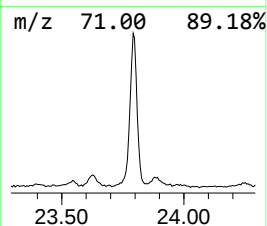
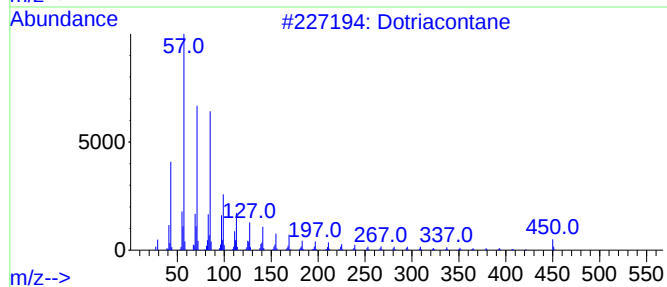
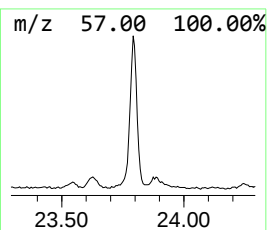
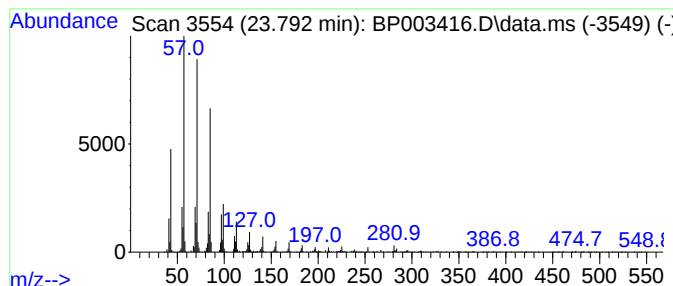
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Dotriacontane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.792	8.18 ng	333606	Perylene-d12	23.251

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dotriacontane	451	C32H66	000544-85-4	96
2			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	96
3			Hexadecane	226	C16H34	000544-76-3	94
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	93
5			2-methyloctacosane	408	C29H60	1000376-72-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP093020\
Data File : BP003416.D
Acq On : 30 Sep 2020 16:39
Operator : CG/JU
Sample : PB131959BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PB131959BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexadecane	20.533	3.5	ng	152933	5	21.057	875416	20.0
Cyclohexadecane	20.786	6.7	ng	292153	5	21.057	875416	20.0
Benzoic acid, 2...	20.839	4.2	ng	182463	5	21.057	875416	20.0
Heneicosane	21.245	2.6	ng	116181	5	21.057	875416	20.0
Heptadecane, 9-...	21.639	2.4	ng	103205	5	21.057	875416	20.0
Heneicosane	22.092	5.3	ng	231831	5	21.057	875416	20.0
Hexadecane, 1-i...	22.592	7.8	ng	317748	6	23.251	815346	20.0
Heneicosane	23.151	9.5	ng	385528	6	23.251	815346	20.0
Dotriacontane	23.792	8.2	ng	333606	6	23.251	815346	20.0